УДК 614.84
Doi: 10.31772/2712-8970-2024-25-3-384-390

Для цитирования: Мозжерин А. В., Паклин Н. Н., Логинов Ю. Ю. Специфика дефектообразования в детекторах на основе теллурида кадмия при импульсном тепловом воздействии // Сибирский аэрокосмический журнал. 2024. Т. 25, № 3. С. 384–390. Doi: 10.31772/2712-8970-2024-25-3-384-390.

For citation: Mozzherin A. V., Paklin N. N., Loginov Yu. Yu. [Specificity of defect formation in detectors based on cadmium telluride under pulsed thermal influence]. *Siberian Aerospace Journal.* 2024, Vol. 25, No. 3, P. 384–390. Doi: 10.31772/2712-8970-2024-25-3-384-390.

Специфика дефектообразования в детекторах на основе теллурида кадмия при импульсном тепловом воздействии

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Активное развитие наукоемких технологий в аэрокосмической отрасли требует рассмотрения работы приборов и устройств в экстремальных условиях, важно исследовать деградацию материалов при быстром нагревании и охлаждении. В данной статье, на основе выполненной теоретической и экспериментальной работы, рассмотрена деградация детекторов на основе теллурида кадмия, вызванная развитием и эволюцией сети точечных дефектов, обусловленных импульсным воздействием с теплодозой около 1000 ºС в течение не более 10 с, имитирующим экстремальную ситуацию короткого замыкания вблизи детектора или прямое нагревание световыми импульсами. Исследование показало, что кристаллический материал в таких экстремальных условиях быстро деградирует вследствие стремительной эволюции дефектной сети. Доработана феноменологическая модель образования и распределения дефектов при кратковременном воздействии теплового излучения на детектор. Электронно-микроскопические исследования образцов, подвергшихся воздействию импульсного инфракрасного излучения, показали развитие плотной дефектной сети, дефектов вакансионного и междоузельного типов, их кластеров и прочих повреждений во всех образцах.

Ключевые слова: теллурид кадмия, точечные дефекты, кластеры дефектов, термическое дефектообразование.

Specificity of defect formation in detectors based on cadmium telluride under pulsed thermal influence

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Active development of science-intensive technologies in the aerospace industry requires consideration of the operation of devices and instruments under extreme conditions; it is important to study the degradation of materials during rapid heating and cooling. On the basis of the theoretical and experimental work *performed, the authors of the paper consider the degradation of cadmium telluride detectors caused by the development and evolution of a network of point defects resulting from pulsed exposure with a heat dose of about 1,000º C for no more than 10 s, simulating an extreme situation of a short circuit near the detector or direct heating by light pulses. The study showed that the crystalline material quickly degrades under such extreme conditions due to the rapid evolution of the defect network. The phenomenological model of the formation and distribution of defects during short-term exposure of the detector to thermal radiation has been improved. Electron microscopic studies of samples exposed to pulsed infrared radiation showed the development of a dense defect network, vacancy and interstitial defects, their clusters and other damage in all samples.*

Keywords: cadmium telluride, point defects, defect clusters, thermal defect formation.

Introduction

The aerospace industry, which is actively developing at present, increasingly faces non-standard tasks arising as a result of the operation of devices and equipment in extreme conditions under pulsed thermal and radiation effects or emergency situations, such as fires and explosions.

Detectors based on cadmium telluride are used as devices for recording pulses of a certain type of radiation [1; 2]. Under certain circumstances, the temperature in the equipment operating area can reach an enormous value, leading to the degradation of materials and, subsequently, the failure of devices and equipment. It is well known that the effect of infrared radiation on a crystalline material leads to the formation and development of a defective structure in it, the evolution of which entails a change in the physicochemical properties. Point defects under the influence of external factors can form clusters that form volumetric defects, which, on the one hand, can lead to the rapid destruction of the material, but on the other hand, up to a certain point, allows it to withstand this destruction. Individual issues of formation and evolution of defects in semiconductors were described earlier in [3–7].

Let us consider an extreme situation when a detector based on cadmium telluride (CdTe) is exposed to extremely high temperatures of 1.000 ºC. Since the melting point of CdTe is 1.092 ºC and the previously mentioned thermal effect is critical for this semiconductor, the limit of its stability in solid-crystal and thin-film samples is of interest.

The aim of the study is to better understand the defect formation processes leading to the degradation of cadmium telluride under short-term pulsed thermal effect with heating up to 1.000 ºC.

Materials, methods and practical results

The object of the study was cadmium telluride, a direct-gap semiconductor of the $A^{II}B^{VI}$ group, one of the promising and actively used materials in microelectronics. The main properties of the material under study are presented in Table 1.

Table 1

Some physicochemical properties of cadmium telluride [5; 8; 9]

Density	5.85 g/cm^3
Melting temperature	1.092 ºC
Solubility in water and other solvents	insoluble
Crystalline structure	cubic, sphalerite (zinc blende)
Lattice parameter	0.648 nm
Poisson's ratio, ν	0.41
Shear modulus	9.2 GPa
Stacking fault energy	11±1.9 mJ/m^2
Fire and explosion safety	incombustible

The CdTe samples were subjected to pulsed action with a heat dose of approximately 1.000 ºC for no more than 10 s, simulating an extreme situation of a short circuit near the detector or direct heating by solar rays. The internal view of the setup and the process of thermal action are shown in Fig. 1.

Рис. 1. Экспериментальная установка и процесс имитации импульсного теплового воздействия

Fig. 1. Experimental setup and process of simulating pulsed thermal action

The experimental part of the study additionally included electron microscopic studies of samples exposed to pulsed infrared radiation to determine the density of the defect network, types of defects, their clusters and other damages. The results obtained showed the presence of a significant defect density in all samples up to 1.019 cm^{-3}. At the same time, the defect density in the thin CdTe film was lower. The defects were represented mainly by vacancies and interstitial atoms, dislocations and dislocation loops, as well as stacking faults (Fig. 2). Additional information on sample preparation and examination on a transmission electron microscope is presented in [5; 10; 11].

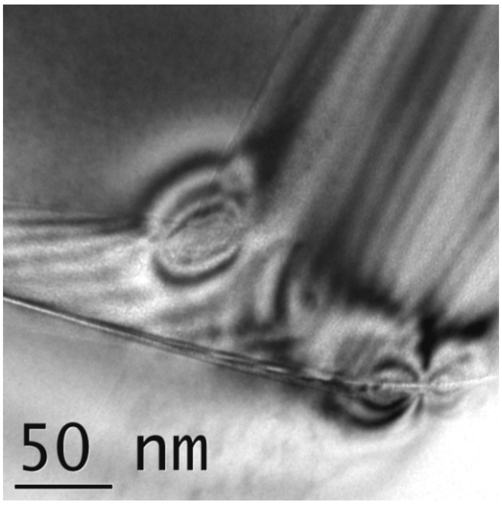

Рис. 2. Формирование дефектов в теллуриде кадмия
после кратковременного теплового воздействия

Fig. 2. Formation of defects in cadmium telluride
after short-term thermal exposure

Model of defect formation in cadmium telluride under pulsed thermal action

The theoretical work was based on the refinement of the mathematical model of physicochemical transformations in CdTe under pulsed action of infrared radiation with an amplitude of 1.000 Cº for no more than 10 s. The pulse was modeled using the formula (Gaussian bell):

$$T = 27\ °C + A \cdot \exp(-t^2),\ \text{where A = 1.000 C°}.$$

The calculation was performed using the Maple mathematical package.

The improved model of physicochemical transformations in semiconductors under the action of thermal radiation was based on a system of modified equations for the evolution of concentrations of structural point and double defects:

$$\frac{\partial n}{\partial t} = P + D_I \frac{\partial^2 n}{\partial z^2} - c_0 R\left(nv + 2nw - 2vm\right) - 2c_0 A_I\left(n^2 + nm\right) + 2Pm, \tag{1}$$

$$\frac{\partial v}{\partial t} = P + D_V \frac{\partial^2 v}{\partial z^2} - c_0 R\left(nv - 2nw + 2vm\right) - 2c_0 A_V\left(v^2 + vw\right) + 2Pw, \tag{2}$$

$$\frac{\partial m}{\partial t} = c_0 A_I\left(n^2 - 2nm\right) - 2c_0 Rvm - Pm, \tag{3}$$

$$\frac{\partial w}{\partial t} = c_0 A_V\left(v^2 - 2vw\right) - 2c_0 Rnw - Pw, \tag{4}$$

where t is the time; z is the distance from the surface to the middle of the film (film thickness is 200 nm). For effective concentrations, the following notations are introduced: C_I and C_V are the concentrations of interstitial atoms and vacancies; C_m and C_w are the concentrations of diinterstitials and divacancies; c_0 is the concentration of ideal cadmium telluride lattice sites. The calculation results are presented in terms of relative concentrations: $n = C_I / c_0$, $v = C_V / c_0$, $m = C_m / c_0$, $w = C_W / c_0$. Notations for model parameters: D_I and D_V are the diffusion (migration) coefficients of interstitial atoms and vacancies; A_I and A_V are the agglomeration (attachment) coefficients of interstitial atoms and vacancies, respectively; R is the recombination coefficient; P is the crystal lattice dissociation coefficient corresponding to the effective energy of thermal Frenkel pair production E_P.

All the listed coefficients are expressed through the activation energies of the reaction as

$$\left(R, A_I, A_V\right) = a^3 \nu \cdot \exp\left(-\frac{1}{kT}\left(E_R, E_I, E_V\right)\right), \tag{5}$$

$$\left(D_I, D_V\right) = a^2 \nu \cdot \exp\left(-\frac{1}{kT}\left(E_{Im}, E_{Vm}\right)\right), \tag{6}$$

$$P = \nu \cdot \exp\left(-\frac{E_P}{kT}\right), \tag{7}$$

here ν is the frequency of oscillations of the crystal lattice; a is the lattice constant; k is the Boltzmann constant; T is the temperature. To solve the equations, it is necessary to take into account diffusion, which affects thin films more significantly than macroscopic samples. The numerical values of the parameters used in expressions (1) – (7) are presented in Table 2.

Table 2

Numerical values of a number of parameters of the CdTe crystal [5; 6; 12–15]

E_{Im}	E_{Vm}	E_I	E_V	E_R	E_P	c_0	ν	a
eV	eV	eV	eV	eV	eV	cm^{-3}	Hz	nm
0.32	0.6	0.45	0.5	0.25	1.4	$1.5 \cdot 10^{22}$	10^{13}	0.648

Solutions of equations (1) – (7) are presented in Fig. 3.

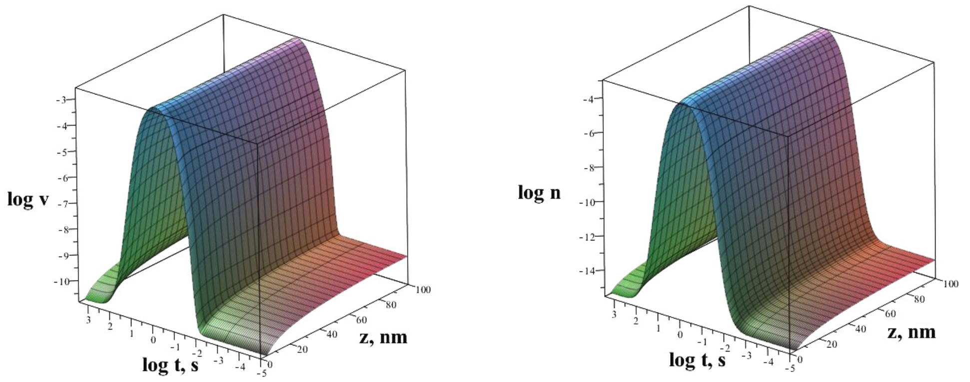

Рис. 3. Зависимость концентраций точечных дефектов (вакансий и междоузлий) от времени и расстояния от поверхности до середины кристаллической пленки при кратковременном тепловом воздействии с амплитудой до 1000 °С

Fig. 3. Dependence of concentrations of point defects (vacancies and interstitials) on time and distance from the surface to the middle of the crystalline film under short-term thermal exposure with an amplitude of up to 1,000 °C

The obtained results (Fig. 3) show good agreement with the experimental data. High temperatures, even acting briefly on cadmium telluride, definitely lead to explosive growth and evolution of the defect network with a concentration of the order of 1.019 cm^{-3} and subsequent destruction of the material. However, studies show that thin-film CdTe samples tend to cool more quickly and reduce the concentration of point defects due to the emergence of some of them on the surface, which reduces the probability of combining into clusters.

Conclusion

A comprehensive study of pulsed thermal effects on a detector made of cadmium telluride was conducted. An increase in detector temperature from 27 to 1.027 ºC was considered. The heating can be caused by exposure to sunlight, infrared radiation during a short circuit near the detector, direct heating of the detector during voltage surges in the power supply network, and pulsed radiation exposure. The study showed that crystalline material quickly degrades under such extreme conditions due to the rapid evolution of the defective network. At the same time, thin-film CdTe samples are more resistant to pulsed thermal effects, and equipment based on them is able to maintain working condition much longer.

The mathematical model, on the basis of which the numerical results were obtained, is a good addition (as an initial condition) to the models describing the evolution of point defects under ionizing radiation.

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Статья поступила в редакцию 30.08.2024; принята к публикации 03.09.2024; опубликована 26.10.2024
The article was submitted 30.08.2024; accepted for publication 03.09.2024; published 26.10.2024