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Original article

Thermal Stability of Cadmium Telluride in Infrared Detectors for Monitoring Fire Conditions

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Abstract

Introduction. Thermal effect of fire on technical means is a common and serious problem. In this regard, it seems an urgent task to study physicochemical and thermal transformations in devices based on cadmium telluride during man-made or natural fires. For a number of materials, such studies have not been conducted, and the available results are insufficient or narrowly focused. The proposed article presents new data on the defect resistance and applicability of the material depending on the thermal effect. The work objective is to study the features of degradation under the influence of extreme temperatures to create new materials with specified properties.

Materials and Methods. Cadmium telluride (CdTe) samples used in solar panels and detectors were studied. In the practical part of the work, the thermal effect on the sample of normal and extreme temperatures was evaluated, followed by the study of the material by transmission electron microscopy methods. The experiments simulated a zone of thermal impact of a fire. The computational and theoretical work consisted in improving the mathematical model of physical and chemical transformations and the evolution of defects under thermal influence up to 1092 °C. The mathematical model took into account the heat dose characteristic of uncontrolled combustion. The Maple software package was used to solve the equations.

Results. The formation of defects in a CdTe sample at significantly different levels of thermal exposure was visualized. The lower limit was about 20 °C, the upper one was more than 600 °C. Transformations in CdTe control samples under the influence of temperatures up to 1092 °C with a step of 15 °C were worked out in detail. Point defects caused by the influence of temperature were presented as a factor of destruction of the material, and consequently, failures in the operation of the device. A system of equations was solved that takes into account a set of parameters: the frequency of vibrations of atoms in the lattice, temperature, concentrations of CdTe nodes, interstitial atoms and vacancies, migration and attachment of interstitial atoms and vacancies. The concentrations of vacancies and interstitial atoms in CdTe samples depending on thickness and temperature were graphically presented. The results of scientific research allowed us to assert that CdTe-based detectors worked relatively correctly only at a heat dose of up to 400 °C. In the ranges of 400-600 °C, the defective network of the material actively evolved, preventing destruction. However, a further increase in thermal exposure led to complete degradation of the equipment, which did not allow the use of cadmium telluride in extreme conditions, even for a short time.

Discussion and Conclusion. The proposed improved model of physical and chemical transformations in CdTe-based devices in heat-affected areas will allow a more selective approach to the use of equipment. In addition, it is necessary to improve materials and increase their resistance to extreme temperatures.

Keywords: cadmium telluride, formation of defects in a CdTe sample, density of nodes, vacancy concentration, CdTe interstitial atoms

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Научная статья

Теплоустойчивость теллурида кадмия в инфракрасных детекторах для мониторинга пожарной обстановки

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Аннотация

Введение. Тепловое воздействие пожара на технические средства — распространенная и серьезная проблема. В этой связи представляется актуальной задачей исследование физико-химических и тепловых превращений в устройствах на основе теллурида кадмия при техногенных или природных пожарах. По ряду материалов подобные исследования не проводились, а имеющиеся результаты недостаточны или узкопрофильны. В предложенной статье представлены новые данные по дефектостойкости и применимости материала в зависимости от теплового воздействия. Цель исследования — изучение особенностей деградации под воздействием экстремальных температур для создания новых материалов с заданными свойствами.

Материалы и методы. Исследовались образцы теллурида кадмия (CdTe), используемые в солнечных панелях и детекторах. В практической части работы оценивалось тепловое воздействие на образец обычных и экстремальных температур с последующим изучением материала методами просвечивающей электронной микроскопии. Эксперименты имитировали зону теплового воздействия пожара. Расчетно-теоретическая работа заключалась в совершенствовании математической модели физико-химических превращений и эволюции дефектов при тепловом воздействии до 1092 °C. Математическая модель учитывала теплодозу, характерную для неуправляемого горения. Для решения уравнений задействовали программный пакет Maple.

Результаты исследования. Визуализировано формирование дефектов в образце CdTe при существенно разных уровнях теплового воздействия. Нижняя граница — около 20 °C, верхняя — более 600 °C. Детально проработаны превращения в контрольных образцах CdTe при воздействии температуры до 1092 °C с шагом 15 °C. Точечные дефекты, обусловленные воздействием температуры, представлены как фактор разрушения материала, а следовательно, и сбоев в работе устройства. Решена система уравнений, которая учитывает комплекс параметров: частоту колебаний атомов в решетке, температуру, концентрации узлов CdTe, междоузельных атомов и вакансий, миграцию и присоединение междоузельных атомов и вакансий. Графически представлены концентрации вакансий и междоузельных атомов в образцах CdTe в зависимости от толщины и температуры. Итоги научных изысканий позволяют утверждать, что детекторы на основе CdTe относительно корректно работают только при теплодозе до 400 °C. В диапазонах 400–600 °C дефектная сеть материала активно эволюционирует, препятствуя разрушению. Однако дальнейшее увеличение теплового воздействия приводит к полной деградации оборудования, что не позволяет использовать теллурид кадмия в экстремальных условиях даже непродолжительное время.

Обсуждение и заключение. Предложенная усовершенствованная модель физико-химических превращений в устройствах на основе CdTe в зонах теплового воздействия позволит более избирательно подходить к вопросу использования оборудования. Кроме того, необходимо совершенствовать материалы и повышать их стойкость к экстремальным температурам.

Ключевые слова: теллурид кадмия, формирование дефектов в образце CdTe, концентрация узлов, концентрация вакансий, междоузельные атомы CdTe

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Introduction. Cadmium telluride (CdTe) is a binary chemical compound of cadmium (Cd) and tellurium (Te), a direct-band semiconductor of the A_2B_6 group. Due to its high melting point and insolubility, it is one of the most stable Cd compounds. CdTe is a strategically important material for creating thin-film solar cells, universal infrared detectors and other devices.

An important issue from the point of view of production practice is the operation of devices and equipment in various environmental conditions, their durability and fire and explosion safety[1]. It is well known that any semiconductor compound tends to degrade and change its physicochemical properties. This is due to the processes of defect formation, which occur, among other things, due to thermal exposure [1]. It is extremely important to understand these processes for the use of materials in extreme conditions while maintaining the specified properties, with minimal risk of fires, accidents and other emergencies.

It should be noted that so far scientific research in this area has not yielded exhaustive results. Studies have not been conducted on a number of materials, and the available data are insufficient or narrow-profile. The authors of the presented article offer new information concerning the resistance to defects and the applicability of the material experiencing thermal effects. The work objective is to study the features of degradation under extreme temperatures to create new materials with specified properties.

Materials and Methods. The operation of the device was studied in the event of extreme events — a natural or man-made fire. The objects of the study were three control samples of cadmium telluride. They were removed from the solar battery and subjected to constant thermal exposure from 20 °C to 1092 °C. Table 1 presents the general data of the studied materials.

Table 1

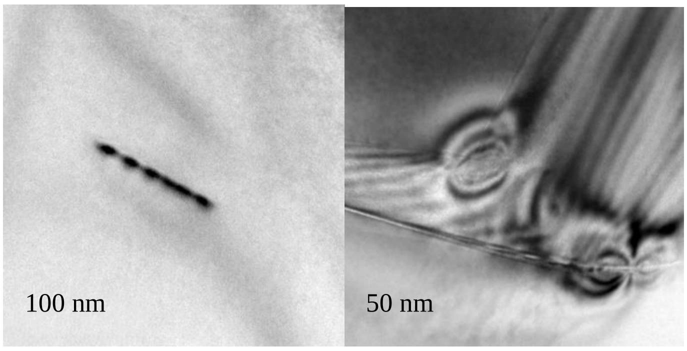
Individual properties and characteristics of cadmium telluride [2–4]

Chemical formula	CdTe
Density, g/cm^3	5.8585
Melting point, °C	1092
Solubility in water and other solvents	Insoluble
Crystal structure	Cubic, sphalerite (zinc blende)
Lattice parameter, nm	0.648
Poisson's ratio, υ	0.41
Shear modulus, GPa	9.2
Stacking fault energy, MJ/m^2	11±1.9
Fire and explosion safety	Incombustible
Toxicity	Toxic, especially dangerous in the aquatic

[1] GOST 2.1.004-91. *Occupational safety standards system. Fire safety. General requirements.* Electronic fund of legal and regulatory documents. URL: https://docs.cntd.ru/document/9051953 (accessed: 17.04.2023).

Basic experimental study was carried out by transmission electron microscopy on a JEOL JEM-2100 device with preliminary sample preparation of samples according to basic techniques [5]. Theoretical work was based on the creation of a mathematical model of physical-chemical transformations in devices based on cadmium telluride, taking into account the heat transfer that occurs during the development of the uncontrolled combustion process. Systems of equations were solved in the Maple software package.

Results. The experimental part of the work was described in [2, 4]. The data obtained showed that the effect of thermal radiation led to the formation and active evolution of a defective network (Fig. 1), represented mainly by growth dislocations. In some cases, in the presence of cadmium or other substances in the atmosphere, precipitates appeared with the transformation of dislocations into dislocation loops or stacking faults [3, 6–7].



a) *b)*

Fig. 1. Formation of defects in the CdTe sample under thermal exposure:
a — ~ 20 °C; *b* — more than 600 °C. Scale in nanometers

Theoretical part of the study included a detailed study of transformations in CdTe control samples when exposed to temperatures up to 1092 °C in increments of 15 °C. With this type of operation of the devices, especially near the melting point, the destruction of the material occurred, which was directly related to the formation and development of point defects.

Taking into account the fixation of the temperature mode and previous experimental data, the formation of interstitial atoms and vacancies, as well as their clusters in the form of dislocation loops and pores in CdTe, was modeled. The effective values of the energy of thermal dissociation of the lattice (E_p) and the coefficient of thermal generation of point defect pairs (P) allowed us to improve the system of equations for the equilibrium distribution of defects, given in [8–9] to the following form:

$$\begin{aligned} Pc_0 + D_I \cdot C_I'' - R \cdot C_I \cdot C_V - 2A_I \cdot C_I^2 = 0, \\ Pc_0 + D_V \cdot C_V'' - R \cdot C_I \cdot C_V - 2A_V \cdot C_V^2 = 0, \end{aligned} \quad (1)$$

where $P = \nu \cdot \exp(-E_p/kT)$, ν — frequency of oscillation of atoms in the lattice, k — the Boltzmann constant, T — temperature, c_0 — concentration of CdTe nodes, C_I and C_V — effective concentrations of interstitial atoms and vacancies, D_I and D_V — diffusion coefficient (migration) of interstitial atoms and vacancies, A_I and A_V — agglomeration coefficient (joining) of interstitial atoms and vacancies, respectively, R — recombination coefficient.

Numerical values of the indicated values were used for calculations (Table 2).

Table 2

Numerical values of the parameters of the cadmium telluride crystal [3, 8–9]

c_0	D_I	D_V	A_I	A_V	R	ν	E_p	P
cm^{-3}	cm^2s^{-1}	cm^2s^{-1}	cm^3s^{-1}	cm^3s^{-1}	cm^3s^{-1}	s^{-1}	eV	cm^3s^{-1}
$1.5 \cdot 10^{22}$	$4.2 \cdot 10^7$	$8.3 \cdot 10^2$	$7.5 \cdot 10^4$	$1.1 \cdot 10^4$	$1.7 \cdot 10^8$	10^{13}	1.4	$2.6 \cdot 10^{-11}$

Solution to system of equations (1) is shown in Fig. 2, 3. As noted above, the upper curve corresponds to 1092 °C, the step is 15 °C.

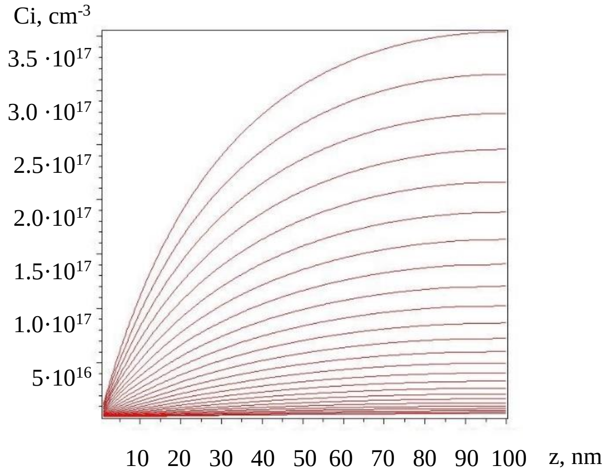


Fig. 2. Vacancy concentrations in CdTe samples depending on thickness (z) at different temperatures

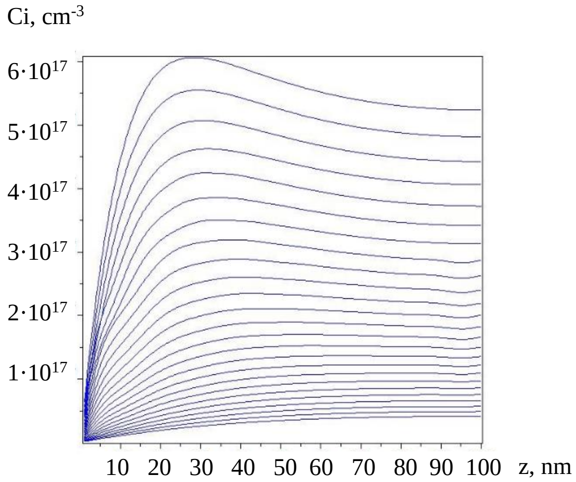


Fig. 3. Concentrations of interstitial atoms in CdTe samples depending on thickness (z) at different temperatures

The data obtained allowed us to assert that up to a temperature of 400 °C, point defects (vacancies and voids) affected the physicochemical properties weakly, with a linear increase. When the specified boundary increased, nonlinear changes were recorded. This could be explained by the reverse effect of defects (countering the destruction of the semiconductor). Active degradation was especially noticeable at temperatures above 600 °C. Under the influence of a temperature of 1000 °C, cadmium telluride began to break down.

Discussion and Conclusion. The presented study confirmed active physical-chemical transformations in cadmium telluride samples at equilibrium thermal exposure up to 1092 °C. The results of solving modified system of equations (1) allow us to assert that with increasing temperature, the destruction in cadmium telluride samples increases, and the defective network grows. These processes cause equipment failure with this material.

Devices and equipment based on cadmium telluride show high thermal stability and reliable operation up to 100 °C. However, their use is limited and becomes extremely ineffective at high temperatures. In extreme conditions, semiconductor materials such as silicon and germanium are more suitable.

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