

# Technology of fabrication of $\text{CdS}_x\text{Te}_{1-x}$ solid solution on silicon substrate

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**Abstract.** Heterojunction between Si and  $\text{CdS}_x\text{Te}_{1-x}$  have been obtained by the method of vacuum deposition of powders of cadmium sulfide and cadmium telluride on the surface of monocrystalline silicon. The optimal temperature regime for the growth of the  $\text{CdS}_x\text{Te}_{1-x}$  solid solution on the silicon surface has been determined. The values of the crystal lattice constant and the thickness of the  $\text{CdS}_x\text{Te}_{1-x}$  solid solution at the interface of the  $n/\text{Si} - n/\text{CdS}_x\text{Te}_{1-x}$  heterostructure are calculated.

## 1 Introduction

Obtaining a heterojunction based on silicon (Si) [1-2] and  $\text{A}^2\text{B}^6$  [3-4] and  $\text{A}^3\text{B}^5$  semiconductor compounds is of scientific and practical interest. This would allow more efficient use of the potential capabilities of the silicon with  $\text{A}^2\text{B}^6$  and  $\text{A}^3\text{B}^5$  semiconductor compounds in solid-state electronics, photovoltaics and photovoltaic energy. In this work certain design issues in the technology of obtaining an efficient heterojunction based on Si and cadmium telluride CdTe without surface states are considered. However, it is known [5] that the crystal lattice constant of silicon ( $\alpha = 5.43\text{\AA}$ ) and cadmium telluride CdTe ( $\alpha = 6.477\text{\AA}$ ) differ considerably, therefore, in order to create an effective heterojunction between these semiconductor materials, it is necessary to use an intermediate semiconductor material that would match their crystal lattice constants. Such a material can be a  $\text{CdS}_x\text{Te}_{1-x}$  solid solution (SS), which is continuous and its lattice constant changes from  $\alpha = 5.84\text{\AA}$  in cadmium sulfide to  $\alpha = 6.477\text{\AA}$  in cadmium telluride. In this solid solution, one can find a composition, in which the lattice constant would correspond to the lattice constant of silicon. For this purpose,  $\text{CdS}_x\text{Te}_{1-x}$  solid solutions of various compositions were formed on the silicon surface.

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For this purpose, CdS and CdTe powders in a weight ratio of 10:1 were placed in a quartz crucible and sprayed onto the silicon surface in a vacuum of  $10^{-5}$  torr. In this case, the source - the crucible was heated in the aisles to the temperatures of  $950^{\circ}\text{C}$  -  $1100^{\circ}\text{C}$ , and the substrate (Si) was at a temperature of  $150\text{-}250^{\circ}\text{C}$ .

## 2 Methods

We created n/Si – n/CdS<sub>x</sub>Te<sub>1-x</sub> heterojunctions by sputtering indium in vacuum of  $\sim 10^{-5}$  Torr with a thickness of  $\sim 400\text{-}500\text{\AA}$  on the surface of high-resistance n-type films with a resistivity of  $\rho \approx 10^5 - 10^6 \Omega \cdot \text{cm}$  with a thickness of  $\sim 4 \mu\text{m}$ .

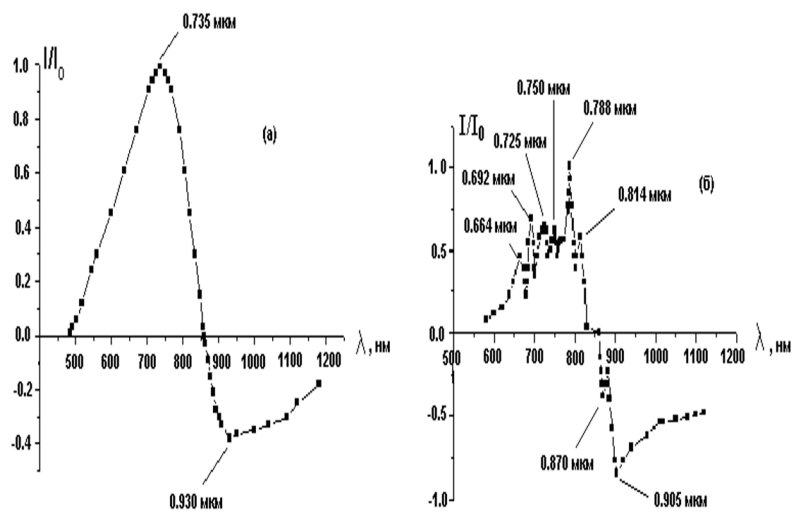
The obtained heterostructures have the most acceptable parameters: no-load voltage and short-circuit current at a temperature of  $t_s = 400^{\circ}\text{C}$ . The n/Si – n/CdS<sub>x</sub>Te<sub>1-x</sub> structures obtained at  $t_s = 465^{\circ}\text{C}$  have electrophysical characteristics, in particular volt-ampere characteristics, as in n-i-n- structures with a long base, where  $d/L = 14\text{-}55$  ( $d$  is a thickness of the i-layer,  $L$  is the diffusion length of minority current carriers).

With an increase in temperature  $t_s$ , the thickness of the CdS<sub>x</sub>Te<sub>1-x</sub> layer increases, and the output parameters of the n/Si – n/CdS<sub>x</sub>Te<sub>1-x</sub> heterostructures deteriorate. Therefore, in this structure, studies were carried out at  $t_s = 400^{\circ}\text{C}$  and  $465^{\circ}\text{C}$ .

The phase composition of the CdS<sub>x</sub>Te<sub>1-x</sub> solid solution was investigated using the photoelectric method. The spectral distribution of photosensitivity was measured in the valve mode on a ZMR-3 monochromator at room temperature. The radiation source was a DKSSh-1000 xenon lamp with a luminous flux of 53000 lm, brightness up to 120 Mcd/m<sup>2</sup> with a central light spot operating in the mode of the minimum allowable power. The radiation is calibrated in absolute units using a thermoelement with an RTE-9 quartz window. The DKSSh-1000 lamp has a continuous spectrum in the UV and visible regions, and powerful radiation lines in the near IR region (800-820 nm). In this method, it is of great importance to establish the sizes of the entrance and exit slits and the resolution of the monochromator, which make it possible to correctly measure the parameters of the sample. The performed estimate showed [6] that the slit width should be  $\sim 10 \mu\text{m}$ . However, in the experiment, a wider slit was set up in order to ensure sufficient photosensitivity of the sample under study, while retaining the possibility of studying subtle phenomena. In this case, the resolution of the monochromator does not exceed 3% in the investigated region of the spectrum.

## 3 Results and discussion

One of the important issues is the study of the composition of the CdS<sub>x</sub>Te<sub>1-x</sub> solid solution. Figures 1a and 1b show the spectral distributions of the photosensitivity of n/Si – n/CdS<sub>x</sub>Te<sub>1-x</sub> heterostructures obtained for structures grown at substrate temperatures  $t_s = 400$  and  $465^{\circ}\text{C}$ . In the spectral distribution of photosensitivity between the intrinsic absorption edges of CdS and CdTe for the n/Si – n/CdS<sub>x</sub>Te<sub>1-x</sub> heterostructure obtained at a temperature of  $t_s = 400^{\circ}\text{C}$ , there are clear peaks  $\lambda_1^{\text{max}} = 0.735 \mu\text{m}$  and  $\lambda_2^{\text{max}} = 0.930 \mu\text{m}$  (Fig. 1a). The spectral distribution of the photosensitivity of the n/Si – n/CdS<sub>x</sub>Te<sub>1-x</sub> heterostructure obtained at a temperature of  $t_s = 465^{\circ}\text{C}$  has several peaks at  $\lambda_1^{\text{max}} = 0.664 \mu\text{m}$ ,  $\lambda_2^{\text{max}} = 0.692 \mu\text{m}$ ,  $\lambda_3^{\text{max}} = 0.725 \mu\text{m}$ ,  $\lambda_4^{\text{max}} = 0.750 \mu\text{m}$ ,  $\lambda_5^{\text{max}} = 0.788 \mu\text{m}$ ,  $\lambda_6^{\text{max}} = 0.814 \mu\text{m}$ ,  $\lambda_7^{\text{max}} = 0.870 \mu\text{m}$ , and  $\lambda_8^{\text{max}} = 0.905 \mu\text{m}$  (Fig. 1b).



**Fig.1.** Spectral distribution of photosensitivity of heterojunctions n/Si – n/CdS, grown at temperatures (a)  $t_s = 400^{\circ}\text{C}$  and (b)  $465^{\circ}\text{C}$

For the detected peaks in the spectral dependence of the photosensitivity distribution, the corresponding fundamental absorption edges  $\lambda_{c.f.a}$  were determined by extrapolating the long-wavelength edge of the photosensitivity maxima to the  $\lambda$  axis. Using the values of the fundamental absorption edges for the detected peaks in the photosensitivity spectrum, the band gap  $E_g$  of solid solutions (SS) formed at the n/Si – n/CdS<sub>x</sub>Te<sub>1-x</sub> heterointerface are determined.

Based on the relationship between the composition of the solid solution and the band gap  $E_g(x)$  [7], the composition of the solid solution CdS<sub>x</sub>Te<sub>1-x</sub> was determined for the found values of  $E_g$ . The determination of the value of the fundamental absorption edge  $\lambda_{c.f.a}$ , the band gap  $E_g$ , and the composition  $x$  of SS for all detected peaks in the photosensitivity spectrum at  $t_s = 400^{\circ}\text{C}$  and  $465^{\circ}\text{C}$  are given in Table 1. The values of the lattice constant  $a_0(x)$  for the detected solid solutions CdS<sub>x</sub>Te<sub>1-x</sub>, which are estimated by the empirical formula  $a_0(x) [\text{\AA}] = 0,6477 - 0,0657x$  [3], are also given in Table 1.

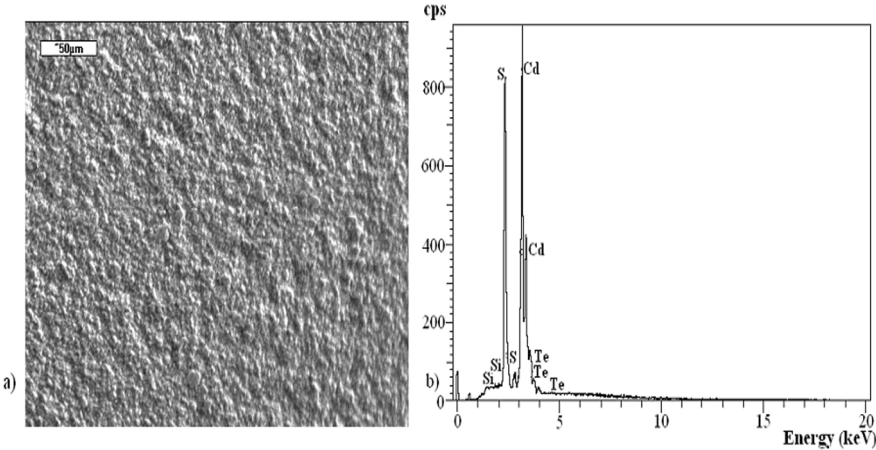
**Table 1.** Dependences of the lattice constant  $a_0(x)$ , average band gap  $E_g^{av}$ , and also fundamental absorption edges  $\lambda_{c.f.a}$  of CdS<sub>x</sub>Te<sub>1-x</sub> solid solution.

$\lambda_{max}, \text{nm}$	$\lambda_{c.f.a.}, \text{nm}$	$E_g, \text{eV}$	$X$	$a_0, (x), \text{\AA}$
664	680	1,82	0,8	5,95
692	718	1,73	0,75	5,98
725	755	1,64	0,69	6,02
750	780	1,59	0,65	6,05
788	802	1,546	0,61	6,13
814	830	1,53	0,56	6,158
735	858	1,44	0,5 0,28	6,192 6,3174
870	881	1,407	0,45	6,2

It should be noted that when determining the composition of  $\text{CdS}_x\text{Te}_{1-x}$  solid solutions with  $E_g = 1.44$  eV using the empirical formula  $E_g [\text{eV}] = 1.74x^2 - 1.01x + 1.51$  [8], the value for  $x$  is obtained in the form of two positive values. For other values of  $E_g$  of SS, only one positive value for  $x$  is obtained. Therefore, in Table 1, for solid solutions with  $E_g = 1.44$  eV, two values of the composition are given, and for other  $E_g$ , one value of the composition  $x$ .

The solid solution with the composition  $x = 0.8$  is closer in composition to the CdS layers, and the solid solution with the composition  $x = 0.28$  is closer to the CdTe layers. The estimate shows that the value of  $a_0(x)$  for Si and SS with a composition of  $x = 0.8$  differ by 8%, and  $a_0(x)$  for CdS and SS films with  $x = 0.8$  differ by only 2%.

Distribution of chemical elements over the surface of obtained layers is investigated. Analyzes were performed on a Jeol - JXA - 8900 microanalytical complex using an EMF LINK ISIS (energy - dispersive spectrometer); error  $\pm 2.0\%$ . Shooting conditions:  $V = 20$  kV,  $I = 10$  nA. Standards: native Cd, Te and Si, for S - synthetic FeS. The measurement results and the microphotograph are shown in Fig. 2 a) and b).



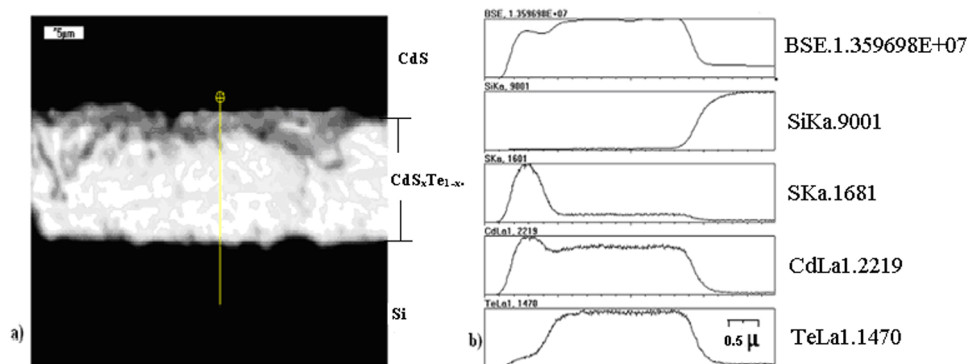
**Fig. 2.** a) Microphotograph from the surfaces of the layers; b) distributions of chemical elements on the surfaces of layers.

As can be seen from Fig. 2b, the emission intensity of the secondary electrons knocked out from the surface layers of the elements of cadmium and sulfide is maximum. This means that the surface of the films mainly consists of cadmium sulfide. The next layer consists of a solid solution of cadmium sulfide and cadmium telluride, then a layer of cadmium telluride and a solid solution of cadmium telluride and silicon (in table 2).

**Table 2.** Quantitative analysis of chemical components of surfaces of (n/Si-CdS<sub>x</sub>Te<sub>1-x</sub>-n/CdS) layers.

Elm t	Spect .	Elem ent	Ato mic	Elmt	Spect.	Element	Atomi c	Elm t	Spect .	Elemen t	Ato mic
	Type	%	%		Type	%	%		Type	%	%
Si K	ED	0.07*	0.20 *	Si K	ED	0.07*	0.17*	Si K	ED	0.03*	0.09 *
S K	ED	20.31	47.0 5	S K	ED	22.34	50.14	S K	ED	22.53	50.5 6
Cd L	ED	78.62	49.3 3	Cd L	ED	77.06	49.33	Cd L	ED	76.74	49.1 4
Te L	ED	1.35	0.79	Te L	ED	0.64	0.36	Te L	ED	0.39	0.22
Tota l		100.3 5	100. 00	Tota l		100.10	100.00	Tota l		99.69	100. 00

Figures 3 a) and b) show microphotographs taken from the cleavage of the layers, as well as the dependences of the distribution of chemical elements on the thickness of the layers. The measurement was carried out at several points.



**Fig.3** a) Microphotographs taken from the cleavage of layer; b) the course of the dependences of the distribution of chemical elements on the thickness of the films.

The results of studies of the dependence of chemical elements on thickness show that in all measured directions the distribution of chemical elements is almost the same and the average spread is no more than  $\sim 5\%$ . Figure 3b also shows the dependences of the layers over the thickness of the films. The top-most microphotograph corresponds to the silicon substrate. The following microphotographs show the distributions of the chemical elements of sulfide, cadmium and telluride in the layers. From the figure it is also possible to estimate the respective thicknesses of each composition. For example, the thickness of cadmium sulfide is approximately one third of the thickness of cadmium telluride (the bump is the third micrograph from the top). The plateau corresponds to the cadmium telluride layer (from the bottom, the second microphotograph on the left side after the crest). It is also possible to estimate the approximate thickness of solid solutions from the figure (decreases in the plot).

## 4 Conclusion

Analyzes of the results obtained show that a solid solution between silicon and cadmium telluride, as well as cadmium telluride and cadmium sulfide is formed with a thickness of  $\sim$  up to 2  $\mu\text{m}$  and  $\sim$  up to 1  $\mu\text{m}$ , respectively (Fig. 3). According to the authors of [5], on the basis of  $\text{A}^2\text{B}^6$  compounds in the  $\text{A}^2 - \text{B}^6$  systems, regions of solid solutions (homogeneity regions) are formed, the length of which can be much larger than that of the  $\text{A}^3\text{B}^5$  compounds. The composition of solid solutions based on  $\text{A}^2\text{B}^6$  compounds can be controlled by setting the conditions for their preparation or processing. Physical and physicochemical properties of solid solutions change with a change in composition, and the nature of the change can be both linear and as well as more complex.

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