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# ANALYSIS OF THE CHANGE IN THE COMPOSITION OF THE CdTe SURFACE UPON IMPLANTATION OF $O_2^+$ IONS AND SUBSEQUENT ANNEALING

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**Abstract.** The methods of implantation of $O_2^+$ ions into a single-crystal CdTe/Mo(111) film followed by annealing at T=800 K for 30 min resulted in the obtained $CdTeO_3$ film. Ion implantation, heating, and investigation of the composition, density of state of valence electrons, and parameters of energy bands are carried out in the same ultra-high vacuum device ($10^{-7}$ Pa). The surface morphology and crystal structure of the oxide are studied using standard scanning electron microscopy and high-speed electron diffraction setups. It has been established that in the valence band of the $CdTeO_3$ film there is a 3rd maximum due to the excitation of electrons from 5s Cd electrons and 2p O electrons and bending 5s Cd + 2pO electrons. Based on the $E_g$ data, it is concluded that quantum size effects are not detected in the case of $CdTeO_3$ films with a thickness of ≥ 30 Å.

***Keywords:*** *$CdTeO_3$, implantation, single-crystal, high-speed, electron diffraction, quantum size.*

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## 1. Introduction

It is known that thin films of $A^{II}B^{VI}$ semiconductors are widely used in the production of multilayer heterostructures used in various optical and electronic devices, solar cells, and photosensitive devices. Thin films of CdTe oxide can have several practical applications; for example, in the production of highly efficient solar cells s (Bube, 1983). Therefore, a large number of investigations are devoted to obtain and study the properties of two and three component structures and multilayer heterostructures based on $A^{II}B^{VI}$ (for example, Me−CdTe−CdS, CdTe-$CdTeO_3$, $SnS_2$/$CdTeO_3$/CdZnTe), (Imanova, 2023; Ali, 2023; Bekpulatov, 2023; Barkaoui, *et al*., 2022). The results of experiments have shown that the perfection and properties of films largely depend on the

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method of synthesis, their thickness, and surface morphology (Normuradov, 2022; Imanova, 2020; Mustafayev, 2015).

It has been shown in investigations (Bekpulatov, 2023) that the chemical composition of the resulting oxide can vary significantly depending on the oxidation conditions before.

Thin films of cadmium telluride oxide were grown by HF method in sputtering an Ar-$N_2O$ atmosphere, and the atomic concentrations of film components were presented as a function of the partial pressure of $N_2O$ in (Garibov, 2014; Umirzakov, 2022; Utanmuraova *et al*., 2023).

The authors presented the film stoichiometry as: $Cd_1^{+2}$ $Te_x^{-2}$ $Te_y^{+4}$ $O_z^{-2}$. Using different index values, representations of several common compounds with these elements are obtained, such as: CdTe ($x = 1$, $y = z = 0$), CdO ($x = y = 0$ and $z = 1$), $CdTeO_3$ ( $x = 0$, $y = 1$ and $z = 3$) and $TeO_2$ ($x = 0$, $y = 1$, $z = 2$ and $z = 3$) and $TeO_2$ ($x = 0$, $y = 1$, $z = 2$ and Cd excluded). Charge neutrality is maintained if the conditions x-2y+z = 1 are satisfied. In several previous works on CdTe oxide, it has been noted that CdTe and $CdTeO_3$ are the main compounds formed, which means that there is a one-to-one stoichiometric ratio between Cd and Te. On the other hand, other previous works on CdTe oxide suggest the possible formation of other compounds, such as $CdTe_2O_5$ (Umirzakov, 2023; Bekpulatov *et al*., 2023).

The low-energy ion implantation method has been widely used for controlled changes in the composition, structure, and properties of semiconductor materials recent years (Umirzakov *et al*., 2022).

The results of an experimental analysis are presented for the preparation of oxide salts on the surface of CdTe (111) films by implantation of $O_2^+$ ions for the first time in this article.

## 2. Methods

Single-crystal samples of CdTe(111) have been used as the object of study. All technological operations (heating, implantation, and studies of the composition and properties carried out) in the same ultrahigh vacuum device ($P \approx 10^{-7}$ Pa) using a set of methods: Auger electron spectroscopy (AES), characteristic energy loss spectroscopy (CELS) and ultraviolet photoelectron spectroscopy (UVPES). The Auger spectra are recorded using an electrostatic analyzer of the Yuz–Rozhansky type with a resolution of 0.2% and small-angle detection of scattered ions and electrons. Oxygen in the ultrahigh vacuum device is let in through an all-metal leak. The gas pressure can be varied within $10^{-2}$ - $10^{-4}$ Pa. At the same time, the pressure in the measuring part of the device did not exceed $10^{-6}$ Pa. The $O_2^+$ ions were obtained by bombarding $O_2$ molecules with electron bombardment. Electrons emitted by the cathode and accelerated by the "cathode-anode" electric field, under the influence of the magnetic field of the solenoid, move along a spiral annular trajectory, and effectively ionize oxygen molecules. These ions are accelerated, focused, and enter the center of the mesh. Since the electron energy was -50 V, the probability of the formation of multiply ionized $O_2$ ions is quite small which can be regulated from $\sim 3$ to $\sim 10$ mm, and current density $O_2^+$ from $5 \cdot 10^{-7}$ to $10^{-3}$ A$\cdot cm^{-2}$. The $Ar^+$ ions are also obtained in a similar way.

The depth distribution profiles of atoms are determined by AES in combination with layer by layer etching with argon ions with $E_0$ = 2 keV at an angle of 5–10° relative to the sample surface. The study of the crystal structure and surface morphology has been carried out in standard setups.

## 3. Results and discussion

Before studying the CdTe/Mo(111) film, it was degassed at $T$ = 800 K for 3-4 hours and briefly at $T$ = 900 K. Figure 1 shows the spectrum of well-purified CdTe(111) single crystals taken by an X-ray diffractometer. The X-ray pattern shows that the cadmium-tellurium film has a cubic lattice, with a constant lattice. It is necessary to note that an increase in temperature to 800 K leads to an increase in the intensity of the peaks. This may be due to the improvement in the crystal structure after an increase in the annealing temperature.

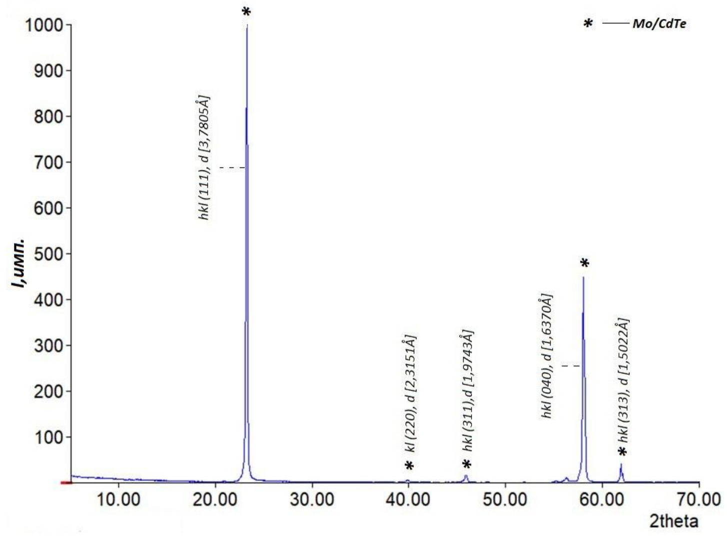


**Fig. 1.** X-ray analysis of CdTe (111)

Figure 2 shows the Auger spectra of the surface of pure CdTe(111) before and after bombardment with oxygen ions with $E_0$ = 1 keV at a saturation dose $D = 6{\cdot}10^{16}$ cm$^{-2}$.

It can be seen that the CdTe(111) spectrum mainly contains intense peaks, Cd, Te, and low-intensity oxygen peaks. After bombardment with $O_2^+$ ions, almost all Auger peaks of impurity atoms disappear, the intensity of the Te and Cd Auger peaks sharply decrease, and intense oxygen Auger peaks appear (Fig. 2, curve 2). In this case, the surface concentrations of Cd, Te, and O were ~19, 22, and 59 at.%, respectively.

After heating at T=800K this system formed a film with an approximate composition of $CdTeO_3$.

The concentration of $C_x$ atoms that make up the film and substrate is determined from the relative change in the intensity of the Auger peaks. The method of coefficients (factors) of elemental Auger sensitivity with matrix corrections is used in the calculations:

$$C_x = \frac{I_x/S_x}{\sum I_i/S_i}\alpha$$

where $I_x$ and $S_x$ are the height of the Auger peak and the elemental Auger sensitivity factor of the $x$th element, respectively; $\sum I_i/S_i$ is the sum of the $I/S$ ratios of all elements present in the sample; α is the matrix correction. The measurement error of the atomic concentration was ~5 at.%. The calculation showed that on the surface of the CdTe film is ~50 at.% Cd, ~48 at.% Te, and O, C atoms, the total concentration of which is ~1.5–2.0 at.%.

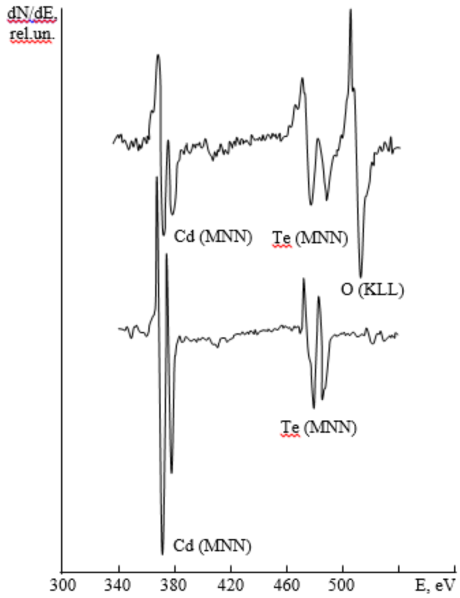


**Fig. 2.** Auger spectra: 1 – pure CdTe (111); 2 – CdTe (111) implanted with $O_2^+$ ions $E_0$ =1 keV at D = $8{\cdot}10^{16}$ cm$^{-2}$

Figure 3 shows the profile of the distribution of oxygen atoms over the depth h of the $CdTeO_3$/CdTe system. It can be seen that up to a depth of 20–25 Å, the oxygen concentration $C_0$ practically does not change, and in the range h ≈ 25–50 Å, it decreases from ~60 at.% to zero. Hence, it follows that the thickness of the $CdTeO_3$ film is ~20-25 Å, and the thickness of the transition layer is ~30 Å.

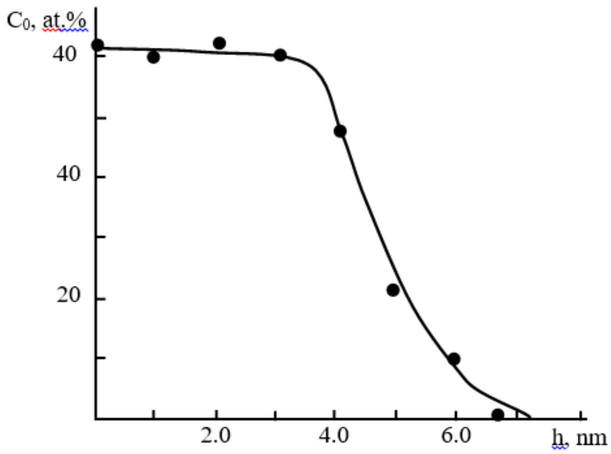


**Fig. 3.** Distribution profile of O atoms over the depth of the $CdTeO_3$/CdTe (111)

Figure 4 shows the SEM and RHEED images of the $CdTeO_3$ film surface. It can be seen that the film surface roughness is ~10–15 Å and has a polycrystalline structure.

Figure 5 shows the spectra of photoelectrons obtained at *hv* = 10.8 eV for and for CdTe with a $CdTeO_3$ film 25-30 Å thick.

The spectrum of pure CdTe (111) exhibits peaks due to the presence of surface states, excitation of Cd 5s electrons, as well as Te 5d and 5s electrons. In the case of a $CdTeO_3$ film, the spectrum shows 3 peaks due to the excitation of 5s Cd electrons, excited electrons from the hybridized state 5sTe + 2pO and excitation of 2p electrons O. Based on the analysis of the spectra of photoelectrons and light absorption, the parameters of the energy bands of CdTe and $CdTeO_3$ are estimated (table) where $E_v$ is top of the valence band, $E_c$ is the bottom of the conduction band, $E_g$ is the band gap (Table 1).

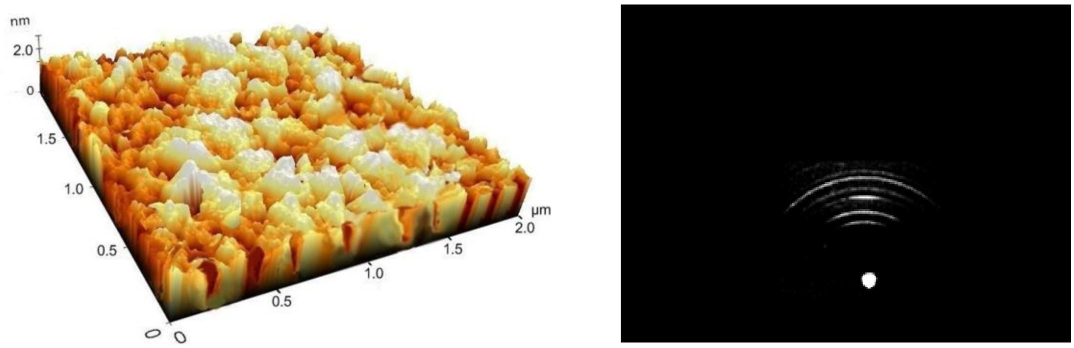


**Fig. 4.** SEM and RHEED images of the $CdTeO_3$ film surface

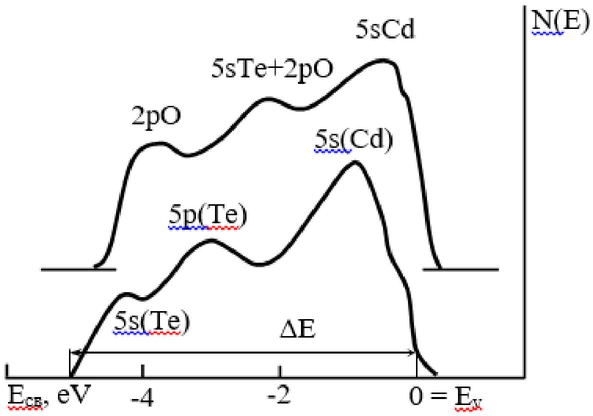


**Fig. 5.** Photoelectron spectra for: 1 – CdTe(111); 2 – CdTe(111) with $CdTeO_3$ film

**Table 1.** Energy Band Parameters of CdTe(111) and $CdTeO_3$

| Pattern | Zone parameters, eV | | |
|---|---|---|---|
| | $E_v$ | $E_c$ | $E_g$ |
| CdTe | 5.65 | 4.20 | 1.45 |
| $CdTeO_3$ | 6.60 | 4.10 | 2.50 |

It can be seen from the table that the $E_g$ of the $CdTeO_3$ film is much larger than the $E_g$ of the CdTe film. It should be noted that the $E_g$ value of the $CdTeO_3$ film obtained by us differs significantly from the $E_g$ value for $CdTeO_3$ nanoparticles given in (Bekpulatov, 2023). Apparently, the $CdTeO_3$ film does not yet exhibit quantum size effects in our case.

## 4. Conclusion

Thus, polycrystalline nano films with a thickness of ~30 to 100 Å have been obtained for the first time by the method of implantation of $O_2^+$ ions in CdTe followed by annealing. The composition, morphology, crystal and electronic structures of the $CdTeO_3$ nanofilm surface are studied. In particular, it is shown that the value of $E_g$ for a $CdTeO_3$ film is ~ 2.50 eV.

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