Properties of the transition layer of the structure of the Schottky barrier Al-CdTe-Mo

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Abstract. The composition and morphology of the n-Al2O3 transition oxide layer at the Al-CdTe interface and the n-MoO3 oxide layer at the CdTe-Mo interface were studied in this work. The Schottky barrier was formed by depositing a polycrystalline p-CdTe layer by a gas-transport reaction in a hydrogen flow onto a Mo substrate. The Schottky barrier was obtained by vacuum deposition of an Al metal layer on the p-CdTe surface. X-ray diffraction phase analysis of the Al-p-CdTe-Mo structure made it possible to establish the real structure, which has the real structure of Al-Al2O3-p-CdTe-MoO3. Based on a scanning electron microscope (SEM), the composition of the Al-p-CdTe structure was studied, where Al is 1.7% Wt, Te is 52.3% Wt, and Cd is 46.0% Wt. The current-voltage characteristics of the Al-CdTe-Mo Schottky barrier in the forward and reverse directions have been studied. The influence of the MoO3 compound layer, which is a wide-gap semiconductor with an n-type orthorhombic structure with a band gap Eg = 2.68 eV, has been revealed. Based on the current-voltage characteristics of the structure, the n-MoO3 layer is determined by smoothing the barrier between the metal and the semiconductor, which affects the mechanism of charge transfer in the structure. The MoO3 compound is a source of electron injection, which is formed during the growth of p-CdTe between the layers of the Mo substrate and the CdTe polycrystalline film. For all samples in the spectral range 190÷900 nm, the absorption edge of Al2O3 films is not observed, which indicates a larger band gap of the oxide Eg ≥ 6.5 eV.

1 Introduction

As studies of recent years have shown, an intermediate layer is formed in a heterogeneous metal-semiconductor system, which can significantly affect the output parameters of the entire structure and is largely determined by the structural and morphological characteristics of the metal, which affect the intensity of diffusion processes and phase formation in transition layers [1-5]. Therefore, further study of the actual structure of a Schottky barrier diode based on pCdTe is not only of scientific but also of practical interest [6].

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Currently, various semiconductor structures based on polycrystalline cadmium telluride (CdTe), which belongs to the A$_2$B$_6$ compounds, are being intensively studied, which are widely used to create detectors of X-ray (X) and γ-radiation [7-10]. The large atomic numbers of the components of this material and the band gap provide a higher efficiency of detection of nuclear radiation by CdTe detectors without cooling compared to Si and Ge detectors [11–13]. Single-crystal CdTe and Cd$_{1-x}$Zn$_x$Te detectors have already shown their advantages over Si-, Ge- and GaAs-detectors and are successfully used in X-ray and γ-ray spectrometry. In recent years, based on CdTe and Cd$_{1-x}$Zn$_x$Te, detectors with a Schottky barrier have been developed [14]. A significant advantage of such detectors is low dark currents (~10$^{-7}$ A against currents of the order of ~10$^{-3}$ A, which increases the operating ranges of the measured energy and sensitivity, leading to a decrease in measurement errors) and high operating temperatures T ≥ 300K, while the above detectors require special cooling for normal operation.

However, single crystals of A$_2$B$_6$ compounds have a number of disadvantages. The main disadvantage of such single crystals is the presence in them of a significant number of defects of various nature, which reduce the lifetime of charge carriers and degrade some of the functional characteristics of the detectors.

Large-block polycrystalline CdTe films with a columnar structure of grains (crystallites) have a number of unique properties [15]. The main advantage of this material is that its crystallites in the direction of vertical growth have the properties of single crystals, and in the horizontal direction—the properties of polycrystals.

The creation and study of semiconductor structures with an extended base, based on polycrystalline CdTe, showed that in the opposite direction, the current remains practically constant when the bias voltage changes over a wide range. This is due to the fact that the active n-Al$_2$O$_3$ oxide layer in the structure is a highly compensated material and the current transfer mechanism is determined by the parameters of recombination phenomena [16], such as the lifetime $\tau$ and the diffusion length $L$ of minority charge carriers.

2 Experiment and discussion of the results

Cadmium telluride films were obtained by resublimation in a hydrogen flow in a quasi-closed volume, which makes it possible to obtain CdTe layers with specified electrical properties. The reverse biased Schottky barrier structure can be used as a detector of short-range nuclear particles, such as alpha particles, nuclear fragments, etc.

The Al–p-CdTe–Mo Schottky barrier was created by thermal deposition of alum (Al) in a vacuum ($\approx$ 10$^{-6}$ Torr) on the surface of p-type large-block CdTe films. The frontal Al contact had a thickness of 80 Å and an area $S \approx 1 \text{ cm}^2$. The molybdenum substrate, whose crystal structure is close in affinity to the CdTe lattice, also served simultaneously as a back contact. The sizes of crystallites in the cross section were from 200 to 250 $\mu$m. The thickness of the p-CdTe films in the structure was 120–170 µm, so that the crystallites penetrated the entire thickness of the film and were almost like a single crystal in the direction of the transfer current. The studies performed have shown that the electrical characteristics of the films are very sensitive to the technological parameters of synthesis [10]. Large-block p-CdTe films were obtained by gas transport epitaxy in a hydrogen flow at atmospheric pressure. The films grown at the substrate temperature $T \approx 650–700 \degree C$ had a resistivity $\rho \approx 2.5 \cdot 10^7$ Ohm·cm. Note that, as the substrate temperature increases, the number of crystallites oriented in the direction of the cubic modification (111) sharply increases [10].

The studies of the X-ray diffraction phase analysis of the Al–p-CdTe–Mo structure (Fig. 1a) made it possible to establish the real structure: Al–Al$_2$O$_3$–p-CdTe–MoO$_3$–Mo.
Fig. 1. Such a structure in its final form is represented as an n-p-n structure (Fig. 1b), where the base (p-CdTe) is in contact on both sides with wide-gap thin oxide layers of n-Al₂O₃ and n-MoO₃.

The authors study the possibility of using aluminum oxide structures as a transparent conducting oxide as a wide-gap n-type semiconductor [16]. Al₂O₃ oxide is widely used in the electronic and electrical industries and, in terms of the combination of electrophysical and economic parameters, is one of the most suitable for the manufacture of installation electrical and radio products. Alumina ceramics finds wide application in the technology of manufacturing substrates for integrated circuits and packages of semiconductor devices. The experiment shows that the resulting Al₂O₃ transition layer transmits optical radiation well in the IR, visible and ultraviolet regions of the spectrum and also [17] in the region of 200÷900 nm the film transmits electromagnetic radiation well. It should be noted that for all samples in the range of 190–900 nm, no absorption edge is observed, which indicates a larger band gap \( E_g \) of Al₂O₃ films than 6.5 eV (Table 1).

Table 1. Parameters of the obtained results of elemental chemical analysis in the Al, Cd, Te elements with the composition Al₂O₃ in the Al-p-CdTe-Mo structure, determined using an energy-dispersive elemental analyzer (EDX (Oxford Instrument)-Aztec Energy Advanced X-act SDD). In the compound, the Al element is 1.7% Wt, Te 52.3% Wt, Cd 46.0% Wt.
A scanning electron microscope (SEM) was used to obtain data on the phase composition, substructure, and morphology of the MoO$_3$ layer (Figure 3). Molybdenum trioxide MoO$_3$ is a promising semiconductor material due to a wide range of interesting properties due to its stoichiometry and preparation methods, including photosensitive and catalytic properties, which find application in electronic display devices, optical storage devices, gas sensors and lithium batteries. Depending on the method of obtaining the Al–p–CdTe–Mo structure in the MoO$_3$ transition layer, the band gap of a direct-gap semiconductor varies in the range of 3.3–3.8 eV. MoO$_3$ transition layers are formed in the process of obtaining the Al–p–CdTe–Mo structure by the gas transport method at the synthesis boundary in a hydrogen flow at the Mo substrate–CdTe layer interface at various substrate temperatures $T_S$, where the source temperature was $T_S = 960 \, ^\circ\text{C}$ (Table 2).
Table 2. Parameters of the obtained results of elemental chemical analysis with the composition $\text{MoO}_3$ of the elements O, Mo, Te in the Al–p–CdTe–Mo structure, determined using an energy-dispersive elemental analyzer.

<table>
<thead>
<tr>
<th>Element</th>
<th>Line type</th>
<th>Conditional concentration</th>
<th>Ratio k</th>
<th>Weight.</th>
<th>Sigma Weight.</th>
<th>Standard name</th>
<th>Preset reference</th>
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<tbody>
<tr>
<td>O</td>
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<td>0.18</td>
<td>0.00060</td>
<td>8.93</td>
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<tr>
<td>Mo</td>
<td>L series</td>
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<td></td>
<td>3.11</td>
<td>0.03112</td>
<td>86.86</td>
<td>0.47</td>
</tr>
<tr>
<td>Te</td>
<td>L series</td>
<td></td>
<td></td>
<td>0.15</td>
<td>0.00114</td>
<td>4.21</td>
<td>0.29</td>
</tr>
</tbody>
</table>

Fig. 4 shows the experimental results of elemental chemical analysis of the composition of the Al–p–CdTe–Mo Schottky barrier structure, determined using an energy-dispersive elemental analyzer.

MoO$_3$ trioxide has the main orthorhombic structure of microcrystals, but the band gap decreases to 2.68 eV and 2.51 eV, respectively, as the substrate temperature increases during the formation of the Al–p–CdTe–Mo Schottky barrier structure. At the highest synthesis temperature of 1100°C, hydrogen and oxygen impurities do not change the layered orthorhombic structure of microcrystals of the MoO$_3$ transition layer, but decrease the band gap to 2.68 eV and 2.51 eV, respectively. The registration of nuclear particles in the detectors occurs in the space charge layers. The geometric dimensions of the space charge, especially its thickness and leakage currents at the rectifying contact, as well as the properties of the ohmic contact, play a decisive role in the formation of the spectrometric parameters of the detectors. Therefore, it is of particular interest to study the electronic processes occurring in the space charge layers formed in the base layers of Schottky barriers with different resistivities. Figure 6 shows the forward and reverse branches of the current-voltage characteristic of a typical Schottky barrier diode (with base...).
$\rho \approx 10^7$ (Ohm·cm) on a semi-logarithmic scale. The forward direction of the current in the structure was considered when a "+" potential was applied to the Mo contact and a reverse "-" potential. A general analysis of the $I$–$V$ characteristics shows that they have rectifying properties and their rectification coefficients, defined as the ratio of forward and reverse current at a fixed voltage $K = \frac{I_{\text{forward}}}{I_{\text{reverse}}}$, are more than four orders of magnitude (Fig. 5).

The $I$–$V$ characteristic consists of four sections, which are described by the following dependences of current on voltage:

1. $I = A V^{\alpha_1}, \alpha_1 = 0.6$;
2. $I = A V^{\alpha_2}, \alpha_2 = 2$;
3. $I = A V^{\alpha_3}, \alpha_3 = 1$;

$\tau_n = \tau_p \approx 10^5 - 10^7$ Ohm·cm. The space charge region thickness $d \approx 5 \mu m$ at $\rho \approx 10^5$ Ohm·cm and $d \approx 30 \mu m$ at $\rho \approx 3 \times 10^7$ Ohm·cm. It has been established that with an increase in the degree of compensation ($\rho$-base), the lifetime $\tau_0$ of equilibrium current carriers increases. For example, when the $\rho$-base increases from $10^5$ Ohm·cm to $3 \times 10^7$ Ohm·cm, the value of $\tau_0$ increases from $4 \times 10^{-8}$ s to $5 \times 10^{-7}$ s.

It is shown that for diodes with a Schottky barrier, made on the basis of large-block p-CdTe films with $\rho \approx 1 \times 10^5$–$1 \times 10^7$ Ohm·cm, even at thermodynamic equilibrium, the space charge has a sufficient thickness: $d \approx 5 \mu m$ at $\rho \approx 1 \times 10^5$ Ohm·cm and $d \approx 30 \mu m$ at $\rho \approx 3 \times 10^7$ Ohm·cm. The study of the current-voltage characteristics of Schottky diodes with the Al-p-CdTe-Mo structure when turned on in the blocking direction showed that after the base of the structure is completely covered by the space charge, electrons are injected from the rear contact, which determine the charge transfer mechanism and the noise characteristics of the structure. Apparently, the MoO$_3$ compound is a source of electron injection, which is formed between the film and the molybdenum substrate, which is formed during the growth of p-CdTe between the Mo and CdTe layers.
3 Conclusions

- Studies show that during the formation of a Schottky barrier, the characteristics of ionizing radiation detectors based on CdZnTe and GaAs:Cr.
- X-ray, gamma, and nuclear radiation detectors based on polycrystalline CdTe and CdZnTe films.

Reference

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