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MECHANISM OF CURRENT PERFORMANCE IN THIN-FILM HETEROJUNCTIONS n-CdS/p-Sb_2Se_3 OBTAINED BY THE CMBD METHOD

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In this work, we analyzed the temperature dependence of the current-voltage characteristics of the structure of glass/Mo/p-Sb_2Se_3/n-CdS/In. From an analysis of the temperature dependences of the direct branches of the I-V characteristic of the heterojunction, it was established that the dominant mechanism of current transfer at low biases (3kT/e<V<0.8V) is multi-stage tunneling-recombination processes involving surface states at the Sb_2Se_3/CdS interface. At V>0.8 V, the dominant current transfer mechanism is Newman tunneling. In the case of reverse bias (3kT/e<V<1.0 eV), the main mechanism of charge carrier transfer through a heterojunction is tunneling through a potential barrier involving a deep energy level. At higher reverse voltages, a soft breakdown occurs.
Keywords: *Sb_2Se_3 SCR; CMBO; Thin films; Heterostructure; Heterojunction*
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INTRODUCTION

Currently, researchers are paying special attention to chalcogenide binary compounds such as Sb_2Se_3, Sb_2S_3, and their solid solutions $Sb_2(S_x,Se_{1-x})_3$ (chemical formula Sb_2X_3) as absorbing layers for solar cells [1]. This interest is due to their favorable physical properties, including p-type conductivity, a band gap (E_g) of 1.1 to 1.8 eV, a high absorption coefficient ($\alpha > 10^5$ cm^{-1} in the visible region of solar radiation), a low melting point (Sb_2Se_3: 823 K, Sb_2S_3: 885 K), and high partial pressure, which are very similar to the properties of Cu(In,Ga)(Se,S) [2]. Additionally, the constituent elements of these materials are relatively inexpensive, abundant in nature, stable under external influences, and non-toxic [3]. These characteristics make it possible to produce environmentally friendly and efficient solar modules, paving the way for their large-scale industrial production.

At present, the efficiency of thin-film solar cells using Sb_2X_3 compounds ranges from 3% to 10.57% [4]. Although these efficiencies are low for large-scale industrial applications, similar to CdTe and Cu(In,Ga)Se-based solar cells, the theoretical maximum efficiency of Sb_2Se_3 solar cells is approximately 32.23% (Shockley-Queisser limit) [5]. Therefore, there is significant potential to improve the efficiency of these solar cells, which have not yet reached their theoretical maximum. The calculated limit values for open-circuit voltage (U_{OC}), short-circuit current (I_{SC}), and fill factor (FF) for Sb_2Se_3 solar cells are U_{OC} = 0.935 V, I_{SC} = 39.99 mA/cm^2, and FF(%) ≤ 87.7%, respectively [5]. To date, the parameters for Sb_2Se_3 solar cells have achieved the following values: U_{OC} = 0.467 V, I_{SC} = 33.52 mA/cm^2, and FF(%) ≤ 67% [6]. Over the past six years, there has been a slight increase in open-circuit voltage and fill factor values. Further improvements in solar cell efficiency can be achieved by increasing these parameters.

In our previous studies, we examined the structural and morphological properties of Sb_2Se_3 films obtained by chemical molecular beam deposition (CMBD) from Sb_2Se_3 powders at different substrate temperatures. The results showed that all films were enriched in antimony, exhibited an orthorhombic structure with predominant orientations (120) and (221), and had crystallite sizes ranging from 200 to 300 nm [7–9].

This study investigates the charge transfer mechanism in thin-film Sb_2Se_3/CdS heterostructures, which primarily determines critical solar cell parameters such as short-circuit current and open-circuit voltage.

EXPERIMENTAL PART

Using the method of chemical molecular beam deposition (CMBD), Sb_2Se_3 films (2–3 μm thick) were obtained on glass substrates with a molybdenum coating. The process of obtaining Sb_2Se_3 solid solution films by the CMBD method is described in detail in [10–12]. Subsequently, thin CdS films (80–100 nm thick) were deposited onto the surfaces of the glass and glass/Mo/ substrates using vacuum deposition. These structures were used to fabricate thin-film glass/Mo/Sb_2Se_3/CdS/In heterostructures.

To enhance the electrical and photovoltaic properties, heat treatments were performed on the glass/Mo/Sb_2Se_3/CdS/In thin-film heterostructures in pure argon at a temperature of approximately 200°C for 30 minutes.

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Indium contacts were then deposited on the front side of the glass/Mo/Sb_2Se_3/CdS/In heterostructures via vacuum deposition. To further improve the front contacts, additional thermal annealing was conducted at a temperature of approximately 200°C for 20 minutes in argon.

The current-voltage characteristics of the glass/Mo/Sb_2Se_3/CdS/In heterostructures were measured using a Keithley SM2460 device. Additionally, the temperature dependences of the current-voltage characteristics at low temperatures (80–300 K) were measured using the van der Pauw method.

RESULTS AND DISCUSSION

Figure 1 shows the forward I-V characteristics of the anisotype p-Sb_2Se_3/n-CdS heterojunction measured at different temperatures. By extrapolating the linear sections of the I-V characteristic to the intersection with the voltage axis, the potential barrier height of the heterojunction at different temperatures was determined (see inset in Fig. 1). It was found that the temperature dependence of the potential barrier height of the p- Sb_2Se_3/n-CdS heterostructure is well described by the equation:

$$\varphi_0(T) = \varphi_0(0) - \beta_\varphi(T)T \, , \tag{1}$$

where $\beta_\varphi = 5.5 \times 10^{-2} \, eV \cdot K^{-1}$ is the temperature coefficient of the potential barrier height, and $\varphi_0(0) = 2.71 \, eV$ is the potential barrier height of the heterostructure at absolute zero temperature (Fig. 2).

It is worth noting that the potential barrier height of the p-Sb_2Se_3/n-CdS heterojunction at room temperature ($\varphi_k = eV_{bi} = 0.84 \, eV$, where V_{bi} is the built-in potential) significantly exceeds the similar parameter for heterojunctions using the semiconductor p-Sb_2Se_3/n-CdS or n-type conductivity ($\varphi_k = 0.3 - 0.4 \, eV$) [13, 14]. The higher potential barrier height of the p-Sb_2Se_3/n-CdS heterojunction is due to the different types of conductivity of the glass and base materials.

The series resistance R_s of the p-Sb_2Se_3/n-CdS heterostructure can be determined from the slope of the forward branch of the I-V characteristic [15]. It can be seen that in the voltage range greater than the height of the potential barrier, the *(I=f(V))* curves (Fig. 1) transform from an exponential dependence to a linear one. This indicates that the voltage across the barrier regions of the heterojunction ceases to change, i.e., the barrier is practically open, and the current through the heterojunction is limited by its series resistance R_s.

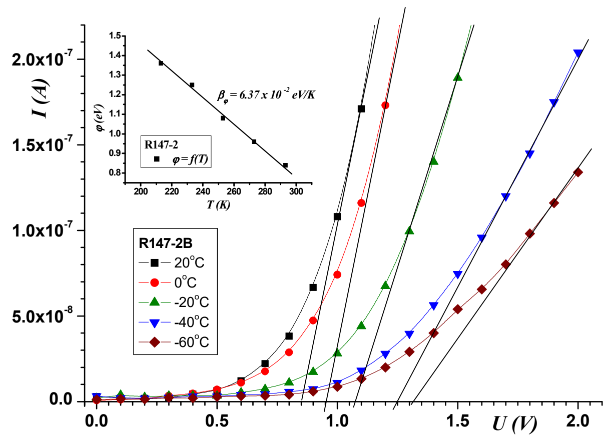

Figure 1. Forward current-voltage (I-V) characteristics of the p-Sb_2Se_3/n-CdS heterostructure at different temperatures (T). The inset shows the temperature dependence of the potential barrier height (φ_0)

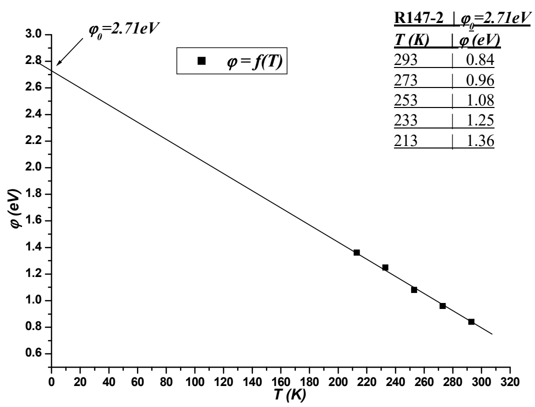

Figure 2. Temperature dependence of the potential barrier height.

To determine the mechanism of current flow, the temperature dependence of the current-voltage (I-V) characteristics of the p-Sb_2Se_3/n-CdS heterostructure was studied. The temperature dependence of the forward branch of the dark I-V characteristic on a semi-logarithmic scale in the voltage range ($kT/e<V<V_D$) is shown in Fig. 3. The I-V characteristic is described by the equation:

$$I = I_{0_1}\exp(eV/A_1\,kT) + I_{0_2}\exp(eV/A_2\,kT). \qquad (2)$$

In the first region, at low voltages $kT/e < V < 0.1\div0.7V$, the exponent of the first exponential is A = 2.21, and in the second region, at higher voltages $0,1\div0,7B \leq V < V_D$ $A_2=1\div1.85.$ ranges from 1 to 1.85. Moreover, the value of the saturation current I_0 decreases with temperature. Therefore, equation (2) can be written as:

$$I = I_0(T)\exp(S_1V) + I_{0_2}(T)\exp(S_2V). \qquad (3)$$

Figure 3 shows the dependence of the forward current on temperature at various voltages on a semi-logarithmic scale. It can be seen that the slope of this dependence dI_{np}/dT does not depend on voltage.

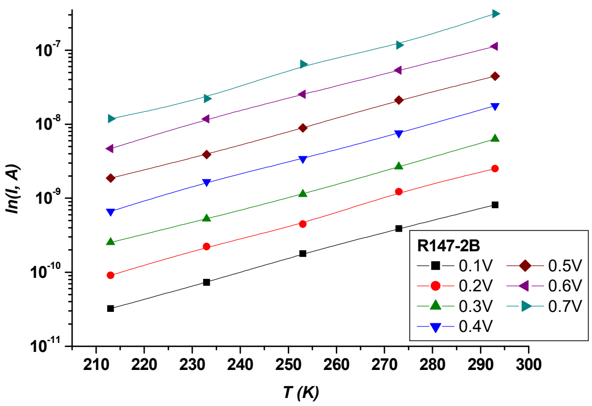

Figure 3. Temperature dependence of the forward current of the p-Sb_2Se_3/n-CdS heterostructure at various biases of 0.1–0.7 V

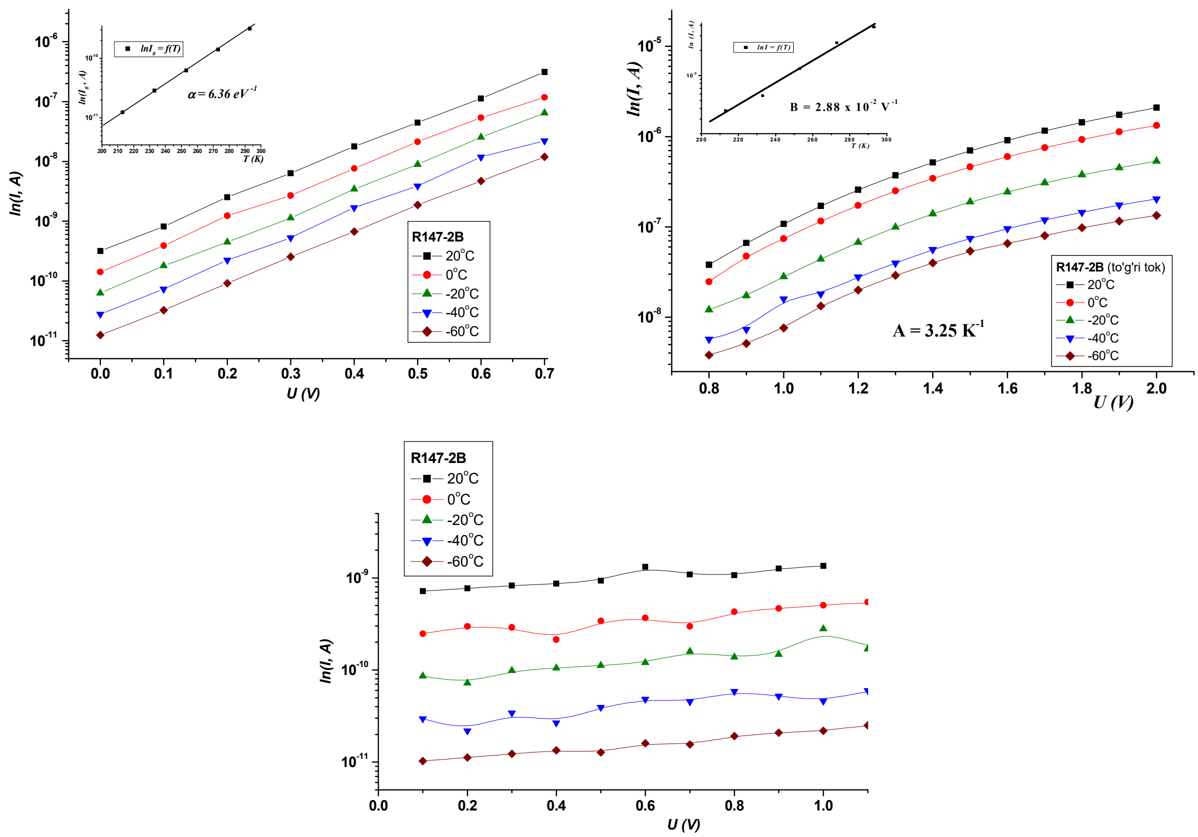

Figure 4. Dark current-voltage characteristics of glass/Mo/p-Sb2Se3/n-CdS/In heterostructures: (a, b) forward current-voltage characteristic, (c) reverse current-voltage characteristic.

Figure 4a shows the forward branches of the current-voltage characteristics of the heterojunction in semi-logarithmic coordinates at different temperatures. In the region of forward biases $V>3kT/e$, straight sections are observed, indicating an exponential dependence of the current on the voltage.

It is worth noting that the slope of the straight sections $(3kT/e<V<0,7B)$ $\Delta ln(I)/\Delta V$ does not depend on temperature. This circumstance excludes the possibility of analyzing current transfer mechanisms based on generation-recombination processes in the space charge region (SCR), since for this case the temperature dependence of the slope of the rectilinear sections of the current-voltage characteristics should be observed in semi-logarithmic coordinates $\Delta ln(I)/\Delta V=e/nkT$, where n is the non-ideality coefficient [16]. The constant slope of the $ln(I)=f(V)$ dependences at different temperatures can be considered as evidence of the tunneling nature of the current transfer mechanism [17, 18].

Straight-line sections of the current-voltage characteristic with identical slopes begin at small displacements, at which the SCR is not yet narrow enough for direct tunneling, which is described by the Newman formula [19]. Therefore, the only physically substantiated current transfer mechanism can be considered multi-stage tunneling-recombination processes involving surface states at the p-Sb_2Se_3/n-CdS interface. In this case, the forward bias current is determined by the following expression [11]:

$$I = B\exp\left(-\alpha(\varphi_0(T) - eV)\right), \tag{4}$$

where B is a quantity that weakly depends on temperature and voltage, and φ_0 is the height of the potential barrier. Rewriting expression (4) in another form:

$$I = B\exp\left(-\alpha(\varphi_0(T)\right)\exp(\alpha eV) = I_0\exp(\alpha eV), \tag{5}$$

where $I_0 = B\exp\left(-\alpha(\varphi_0(T)\right)$ is the cutoff current, which does not depend on the applied voltage. From expression (4) it is clear that the slope $\Delta ln(I)/\Delta V$ of the initial sections of the forward branches of the current-voltage characteristic, shown in Fig. 4a, determines the coefficient α, which takes a value of 3.6 eV^{-1}.

From the current-voltage characteristics presented in Fig. 4b, we can qualitatively conclude that the predominant mechanism of carrier transfer in the studied heterostructure is tunneling, and it is described by the empirical formula:

$$I = I_0\exp(AT + BV), \tag{6}$$

where A and B are experimentally determined quantities that are typical for the tunnel-recombination mechanism of current passage in the heterostructure. Based on the calculation results, it was determined that $A=3,25\ K^{-1}$ and $B=2.88\times10^{-2}\ B^{-1}$.

The mechanism of current passage at reverse biases $kT/e<V<1.0$ is due to the thermal generation of charge carriers in the SCR (Fig. 4c). At higher reverse biases 1<V<5 V, the tunnel charge transfer mechanism predominates.

CONCLUSION

Thin-film heterostructures based on Sb_2Se_3 films on borosilicate substrates coated with a molybdenum layer using the CMBD method were obtained. The results of measuring the current-voltage characteristics of the heterostructures showed that after heat treatment, the main parameters (k, φ_0, R_s) of thin-film glass/Mo/Sb_2Se_3/CdS heterostructures improved and had the following values: $k\approx1\cdot10^{2\div3}$, $R_s=80\ \Omega$, $\alpha=6.36\ eV^{-1}$, $A=3.25\ K^{-1}$ and $B=2.88\times10^{-2}\ V^{-1}$, $\beta_\varphi=5.7\cdot10^{-2}\ eV/K$, $\varphi\approx0.84\div0.95\ eV$, $\varphi_0=2.71\ eV$, $\varphi=0.4\div0.45\ eV$, which will make it possible to produce efficient solar cells based on them.

From an analysis of the temperature dependences of the direct branches of the I-V characteristic of the heterojunction, it was established that the dominant mechanism of current transfer at low biases ($3kT/e<V<0.8$V) is multi-stage tunneling-recombination processes involving surface states at the Sb_xSe_y/CdS interface. At $V>0.8$B, the dominant current transfer mechanism is Newman tunneling. In the case of reverse bias ($3kT/e<V<1.0$ eV), the main mechanism of charge carrier transfer through a heterojunction is tunneling through a potential barrier involving a deep energy level.

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МЕХАНІЗМ ПРОТІКАННЯ СТРУМУ В ТОНКОПЛІВКОВИХ ГЕТЕРОПЕРЕХОДАХ n-CdS/p-Sb_2Se_3, ОТРИМАНИХ МЕТОДОМ CMBD

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У даній роботі проаналізовано температурну залежність вольт-амперної характеристики структури скло/Mo/p-Sb_2Se_3/n-CdS/In. З аналізу температурних залежностей прямих гілок ВАХ гетеропереходу встановлено, що домінуючим механізмом передачі струму при малих зміщеннях (3kT/e<V<0,8V) є багатоступінчасті тунельно-рекомбінаційні процеси. за участю поверхневих станів на межі розділу Sb_2Se_3 /CdS. При V>0,8 В домінуючим механізмом передачі струму є тунелювання Ньюмена. У випадку зворотного зсуву (3kT/e<V<1,0 еВ) основним механізмом перенесення носія заряду через гетероперехід є тунелювання через потенційний бар'єр із залученням глибокого рівня енергії. При більш високих зворотних напругах відбувається м'який пробій.

Ключові слова: *Sb_2Se_3 SCR; CMBO; тонкі плівки; гетероструктура; гетероперехід*