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# Physical properties of the films $\text{Bi}_2\text{Te}_3\text{-Bi}_2\text{Se}_3$ and thermophotovoltaic elements on their basis

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**Abstract:** As a result of work are received p-n heterojunctions in thin-film execution, described by high values of differential resistance. Results of researches show, that film p-n the structures received by a method of discrete thermal evaporation in a uniform work cycle, are suitable for use in low-voltage devices. The effect of conditions of precipitation on clarifying properties  $\text{SiO}_x$  of surface slicks for thermophotovoltaic elements on a basis  $\text{Bi}_2\text{Se}_3$  and  $\text{Bi}_2\text{Te}_3$  is probed. The comparison with values of a current density of short-circuit raw of thermophotovoltaic elements is conducted. The augmentation of a current density with body height of concentration of oxygen in a mixed gas is exhibited during precipitation of a film that is explained by smaller absorption of a light in a film. For the maximal augmentation of a current of short-circuit of thermophotovoltaic elements the optimum thickness of optical stratum is defined.

**Keywords:** Thin Film, P-N the Structures, Component, Thermophotovoltaic Elements, Surface

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## 1. Introduction

The volt-ampere and volt-farads characteristic in an interval of temperatures 77-300K are investigated. With this purpose the structure p- $\text{Bi}_2\text{Te}_3$  - n- $\text{Bi}_2\text{Se}_3$  also was mounted in vacuum cryostat, where furnace and the sensor of temperature were in a landing place of a sample. The temperature regulator provided maintenance of temperature with accuracy  $\pm 1^\circ\text{C}$ .

Breezy samples possessed straightening properties; the factor of straightening on occasions reached value  $10^2$  at displacement 0,2V and temperature 80K. Straightening character volt-ampere characteristic is kept down to temperature 300K.

With increase in temperature direct currents are limited to more high-resistance layers  $\text{Bi}_2\text{Te}_{3-x}\text{Se}_x$  heterojunction, reverse currents grow more intensively and consequently at temperatures  $T > 200\text{K}$  the factor of straightening appreciably decreases.

At voltage more than 30mV straight lines volt-ampere characteristic are described by function of a kind  $I = I_0 \exp(qV / \beta kT)$ , with factor of ideality  $\beta = 2-2,5$  characteristic for a current, limited recombination's of carriers in a layer of a volumetric charge. The size  $\beta$  increases up to 3

at 100K.

At the big voltage linear dependence  $I(V)$  operates. The size diffusion's site of the volt - ampere characteristic in the field of the big currents makes 0,095-0,100V.

In temperature dependence of an inclination of straight lines  $\ln I \equiv V$  three intervals of temperatures are allocated: 77-100; 100-200; 200-300K.

With growth of temperature is higher 100K an inclination changes, and is lower 100K remains to constants, and at temperatures 77-100K initial sites of the volt-ampere characteristic is not described by expression  $I = qSNd \exp[-q(V_{D_n} \cdot V)]$ . Temperature dependence of a current on a voltage is much weaker, than it is necessary to expect from generations-recombination's model. In a temperature range (77-100K) had a constant inclination (fig. 1, curves 1-3) more often, and the exponential site was well described by expression, characteristic for a tunnel current  $I = I_0 \exp(BT) \exp(AV)$ , where  $A$  and  $B$  - constants, not dependent on temperature and voltage, which sizes were in limits  $A = 12-15\text{V}^{-1}$ ,  $B = (2-5) \times 10^{-2}\text{K}^{-1}$ .

In this case Fermi's levels lay in a zone of conductivity and in a valent zone accordingly for n- $\text{Bi}_2\text{Se}_3$  and p- $\text{Bi}_2\text{Te}_3$ . It allows assuming, that at low temperatures the prevailing

mechanism of passage of a current through structures is tunneling carriers "zone - zone". Weak temperature dependence of a direct current, constancy  $dI/dV$  at change of temperature and great value of a current of saturation specifies such opportunity. At high temperatures the tunnel current also exists, but because of stronger temperature dependence a generations-recombination's current tunneling gives the small contribution to the common current.

## 2. Data Collection and Analysis

Hence, in the field of temperatures (100-200K) course of a current is limited to a generations-recombination's current on border of the unit (fig. 1, curves 4-6). At higher temperatures (200-300K), prevailing become activity processes. The inclination a exponential site became temperature-dependent, experimental points well to be lying on straight lines in coordinates  $\ln I \cong T^{-1}$ .

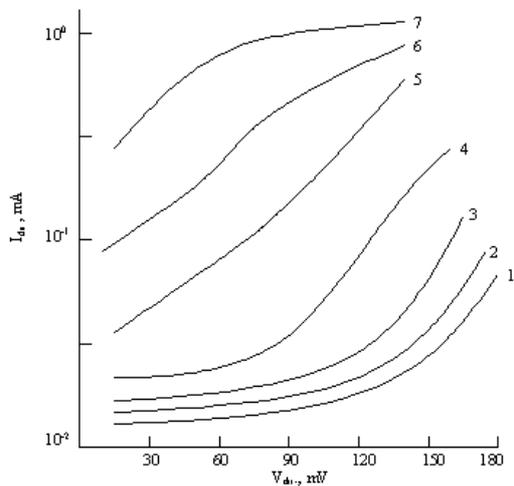


Figure 1. Dependence of direct currents on the enclosed voltage at various temperatures. (1 - T=77K; 2 - T=90K; 3 - T=100K; 4 - T=130K; 5 - T=160K; 6 - T=220K; 7 - T=300K)

Proceeding from the tunnel mechanism of carry of a current, in double logarithmic scale dependence of a current on a voltage can look as sedate. At small displacement (20-30mV) reverse branches submit to the sedate dependence, which can be connected to presence of superficial outflow or the complex mechanism of tunneling [1, 2].

From temperature dependence of a reverse current (for various displacement) it is possible to draw a conclusion, that in the field of temperatures 100-200K course of a current is defined by a generation's current, since at voltage 30-200mV the reverse current has the sedate dependence close to  $kI \cong V^n$ , ( $n \approx \frac{1}{2}$ ) which is characteristic for a generation's current for a case of sharp transition.

As the reverse current with growth of a voltage changes under the reverse law  $I_{o\partial p} \cong \sqrt{V}$ , at 30-130mV direct displacement the direct current is described by dependence  $I = I_0 \exp(qV / \beta kT)$ , where  $\beta \sim 2$ . Thus, it is possible to

conclude, that in an interval 77-130K at  $V_{direct} = 20-130mV$  and  $V_{reverse} = 40-120mV$ . Thus the reverse current through transition is basically generations, and a straight line – recombination.

At temperatures from above 200K, the exponent becomes more than 1.

Measurement of capacity p-n transition depending on a voltage allows to determine such major parameters, as the width of area of a volumetric charge, diffusion potential, concentration of acceptors and donors in the field of a volumetric charge, structure of a locking layer, the mechanism of straightening, etc.

Results of measurements testify to sharpness of transition of the volt - farad characteristic resulted on fig. 2.

As is known for a barrier the metal - semiconductor, as well as for sharp asymmetrical transition, the width of the impoverished layer is expressed by the following formula

$$W = \sqrt{2\epsilon_S(V_B - V - kT)q / N_d} \quad (1)$$

The specific capacity of the impoverished layer is defined by the formula

$$C = \sqrt{q\epsilon_S N_d (2(V_B - V - kT)q)} \quad (2)$$

Whence

$$N_d = (2/q\epsilon_S) \left[ -1 / (d(1/C^2) / dV) \right] \quad (3)$$

The analysis of the volt - ampere characteristic of structures Bi<sub>2</sub>Te<sub>3</sub> – Bi<sub>2</sub>Se<sub>3</sub> carried out. The schedule of dependence on negative voltage is constructed. Apparently from figure 2 dependence  $C^{-2} \cong V$  has linear character up to 0,1V. Concentration ionized centers  $N_d$  in a barrier, determined on an inclination  $C^{-2} \cong V$  makes  $4 \cdot 10^{15} cm^{-3}$ .

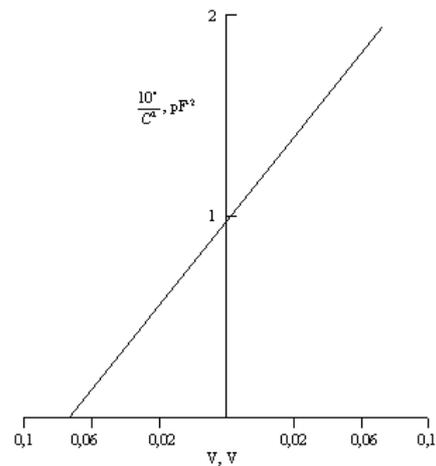


Figure 2. The volt - farad characteristic of structure p-Bi<sub>2</sub>Te<sub>3</sub> - n-Bi<sub>2</sub>Se<sub>3</sub>

The diffusion potential determined by extrapolation of resulted dependence is equal  $\sim 0,08-0,09V$ .

Influence of an intermediate layer on capacity is in details analyzed on the basis of Bardin's model [3]. At presence of a thin high-resistance layer by superficial charges on border

undressed dependence  $C^{-2}$  from  $V_{reverse}$  remains still linear with an inclination  $2/qeN_d$ , as well as for the diode without an intermediate layer, but the point of crossing of this dependence with axis  $V_{reverse}$  is displaced aside higher values.

In the major parameter describing qualitatively made structures, the size of differential resistance is at zero displacement. The experimental points reflecting dependence of differential resistance at zero displacement from temperature are shown on fig. 3. Apparently, the resulted dependence submits to the exponential law in an interval of temperatures 77-200K, and at high temperatures dependence amplifies.

Efficient and technologically advanced method of increasing power generation thermophotovoltaic elements is to apply on their front surface antireflection films, which are at the same time can serve as protective coatings and passivation [4]. Pure silicon is polished reflects more than 30% of the incident solar radiation. For conventional silicon intensive research optimal antireflection coating. Proposed use as antireflection coatings for solar cells based on silicon materials such as ZnS [5], Ta<sub>2</sub>O<sub>5</sub> [6], Si<sub>3</sub>N<sub>4</sub> [7], SiO<sub>x</sub> [8, 9], SnO<sub>2</sub> [10], Nd<sub>2</sub>O<sub>3</sub> [11] and others. Including works [6] showed the possibility of making use of a different and dual-layer optical films. Advantage over other SiO<sub>x</sub> antireflection coatings is their ease of deposition methods, as well as the ability to change their optical properties in a wide range by changing the oxygen content.

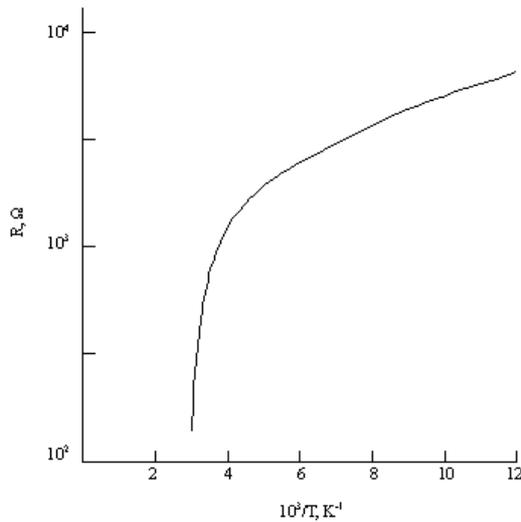


Figure 3. Temperature dependence of differential resistance at zero displacement.

SiO<sub>x</sub> films were prepared by spraying the element thermophotovoltaic argon - oxygen mixture. Oxygen and argon were presented in volume of the chamber through a vacuum tee with two needle inlet valve having a solenoid valves to override the gas flow into the chamber. Feed gas pressure and adjusting them as follows: for each of the needle through the inlet valve pressure reducers 5x10<sup>5</sup>Pa fed gas from two cylinders filled with oxygen and argon. After pumping the

spray chamber to a high vacuum (2,3x10<sup>3</sup>Pa) opened solenoid valve inlet valve of the oxygen line and the working volume of supplied oxygen pressure in the chamber is regulated by a needle inlet valve. Then oxygen inlet valve solenoid valve overlap, the working volume again evacuated to a high vacuum solenoid valve opens and argon inlet valve after installation argon pressure solenoid valve opens the oxygen line. In this case, the camera sets the necessary pressure argon - oxygen mixture. This allows to obtain an effective antireflection coating for thermophotoelements altering the partial pressure of the gas mixture in the reaction chamber and the gas mixture during the deposition [11]. These films can simultaneously serve as the quality of protective coatings and passivation. In this paper theoretically calculated effect of oxygen on SiO<sub>x</sub> antireflection properties with respect to the silicon thermophotovoltaic elements. Calculations were performed for SiO<sub>x</sub>, silicon deposited on the substrate by methods as described in [12]. Spectral dependence of the refractive index and absorption coefficient SiO<sub>x</sub> be determined in the range 0.4-1.4 microns. We present the corresponding data for the films obtained at different oxygen content in the gas mixture (Fig. 4.).

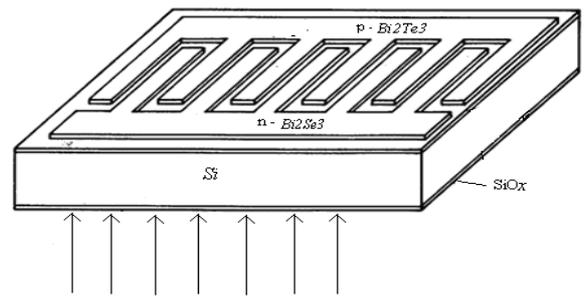


Figure 4. Structural diagram thermophotovoltaic element with antireflection layer SiO<sub>x</sub>.

Illumination thermophotovoltaic elements assessed by an increase in short-circuit photocurrent, according to the formula [6]:

$$I = q \int_{\lambda_{min}}^{\lambda_{max}} F(\lambda)T(\lambda)Q(\lambda)d\lambda \quad (4)$$

where  $q$  - electron charge,  $\lambda_{max}$  and  $\lambda_{min}$  - upper and lower bounds of wavelengths,  $F(\lambda)$  - the spectral intensity of solar radiation,  $T(\lambda)$  - the coefficient of transmission and anti-reflective coating,  $Q(\lambda)$  - quantum yield of element. To study the reflection properties of SiO<sub>x</sub> films, one can assume that the quantum yield is unity in all calculations, i.e. each photon creation the electron - hole pair. In this model, the upper limit of photon sensitivity for thermophotovoltaic element equal to 1.4 microns, 0.4 microns lower limit, since at smaller wavelengths photoconversion efficiency abruptly decreases by [10].

### 3. Results and Discussion

Calculations of the spectral dependences of the coefficients of reflection and transmission SiOx films on a silicon substrate used the formulas of this optical model [12]. Were taken into account the spectral dependence of the refractive index and absorption coefficient of silicon. To determine the optimal thickness of the optical layer with the best anti-reflective effect of the problem of finding the maximum short-circuit current (4) was solved by numerical method by dividing the wavelength range from minimum to maximum on  $\Delta\lambda$ .

Least reflection from the front surface thermophotovoltaic element is achieved when the refractive index of the film is the square root of the refractive index of silicon. In the case of non-absorbing antireflective film reflection minimum coincides with the maximum transmittance of light in the active layer thermophotovoltaic element. In the studied spectral range of the average value of the refractive index of silicon is 3.85, which means the maximum antireflection effect is achieved at a value  $\sqrt{3,85}=1,96$  in the case of weakly absorbing coating. Reflection of light from the front surface of the element determines thermophotovoltaic photoconversion efficiency. A film deposited from a gaseous mixture with an oxygen content of 0.5, an average refractive index closest to an optimal value. As the concentration of oxygen during film deposition average value of the refractive indices decrease. Thus, the short circuit current thermophotovoltaic elements SiOx coated films should decrease with increasing oxygen concentration in the gas mixture during the deposition of the films.

Fig. 5 shows the dependence of the integral short-circuit current densities thermophotovoltaic elements coated SiOx films deposited from gas mixtures with different oxygen concentrations. Values of the integral short-circuit current thermophotovoltaic elements increase with increasing oxygen concentration in the gas mixture during the deposition of anti-reflective coatings.

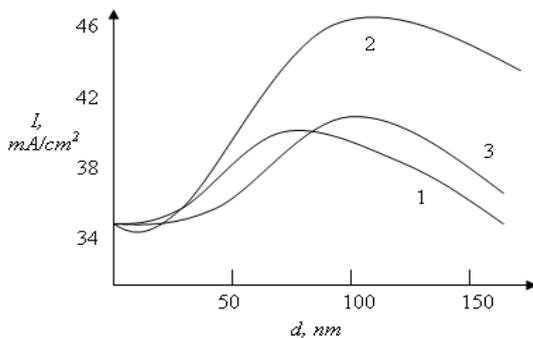


Figure 5. Integral photocurrent density thermophotovoltaic elements depending on the thickness of an antireflection coating for Si-Ox films deposited from gas mixtures with a different content of nitrogen: 1 - 0.5; 2 - 1.0; 3 - 2.0.

Current value increases to 1.1 times the coating deposited from a gaseous mixture with oxygen  $x = 0.5$ , and 1.3 times – with  $x = 1.0$  oxygen, compared with the thermophotovoltaic

element uncoated.

Behavior of the short circuit current is determined not only by light reflected from the front surface of the optical film, but also by absorption in its entirety. This assumption is supported by fig. 3, which shows the dependence of the reflection coefficients of transmission of the films deposited from a gaseous mixture with an oxygen content of  $x = 1.0$ , the optimal thickness.

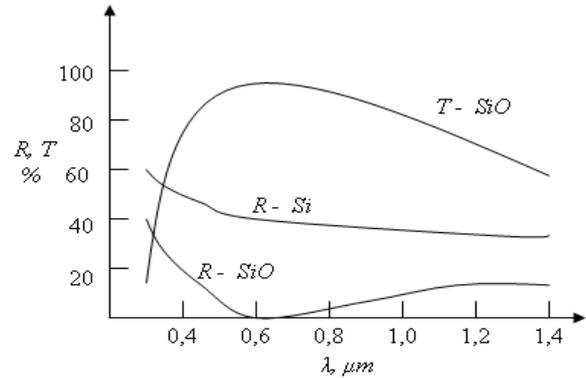


Figure 6. Wavelength dependence of the reflection coefficients (R - SiO) and transmittance (T - SiO) films deposited from the gas mixture. (R - Si) - spectrum reflected from the surface of pure silicon.

Films deposited from a gaseous mixture with oxygen  $x=1.0$ , have a minimum reflectance in the wavelength region of 0.6-1.0 micrometers. However, due to increasing the absorption of light in the film grown at lower concentrations of oxygen and light transmission decreases. Hallmark of SiOx as optical coatings remains the possibility of varying the oxygen concentration when applying optical films and management of optical parameters that can be used in the formation of effective anti-reflective coatings for thermophotovoltaic elements.

### 4. Conclusion

As a result of work are received p-n heterojunctions in thin-film execution, described by high values of differential resistance. Results of researches show, that film p-n the structures received by a method of discrete thermal evaporation in a uniform work cycle, are suitable for use in low-voltage devices.

The effect of conditions of precipitation on clarifying properties SiOx of surface slicks for thermophotovoltaic elements on a basis Bi<sub>2</sub>Se<sub>3</sub> and Bi<sub>2</sub>Te<sub>3</sub> is probed. The comparison with values of a current density of short-circuit raw of thermophotovoltaic elements is conducted. The augmentation of a current density with body height of concentration of oxygen in a mixed gas is exhibited during precipitation of a film that is explained by smaller absorption of a light in a film. For the maximal augmentation of a current of short-circuit of thermophotovoltaic elements the optimum thickness of optical stratum is defined.

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