Monocrystals Ag_3SbS_3: Investigation of electrical characteristics

G.Khlyap[a*], V.Belosertseva[b], L.Panchenko[c], M.Andrukhiv[a]

[a] State Pedagogical University, 24 Franko str., Drogobych 82100,UKRAINE
[b]Kharkiv State Politechnical University, 21 Frunze str., 61002 Kharkiv, UKRAINE
[c]Sumy State University, 2 R.- Korsakov str., Sumy 244007, UKRAINE

ABSTRACT

Electrical characteristics (current-voltage and capacitance-voltage) of metal-semiconductor structure based on monocrystals Ag_3SbS_3 are reported. Studies carried out at the room temperature were shown space-charge limited (SCL) current caused by the peculiarities of Ag_3SbS_3 crystallographic structure: velocity saturation mode and ballistic regime were observed. Results of the numerical modeling of experimental data are also presented.

Keywords: Ag_3SbS_3 monocrystal, I-V and C-V measurements, SCL-current, numerical modeling.

1. INTRODUCTION

Recently, the attention of researchers has been attracted by chalcogenide semiconductor systemas $A^1B^5C^6$. The compound Ag_3SbS_3 (pyrargyrite) is of particular interest. Due its high electrooptical effect, significant double-beam refraction and transparency in the wave length 0.6-14 μm, this material is very important for many technical applications. However, the electrical characteristics of the compound and structures based on this material have been poorly studied so far. The article reports first results of electric studies of barrier structure metal-semiconductor based on p-Ag_3SbS_3 compound.

2. Ag_3SbS_3 MONOCRYSTALS STRUCTURE

This compound belongs to the crystallographic group R3C (C_{3v}^6); Z=6; a = 11.04 Å, c = 8.72 Å. The rhombohedron cell formes the structure basis: a = 7.01 Å, α = 104°04 with trigonal piramids SbS_3 at the apex and in the centre of the rhombohedron[1] . Fig. 1 plots the scheme of pirargyrite elemental cell One of the peculiarities of the crystallographic structure is the availability of infinite spiral-like chains ...S – Ag – S ... formed along Z axis.

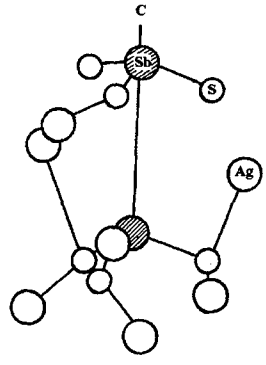

Fig.1. Crystallographic elemental cell of Ag_3SbS_3.

Further author information –
G.K.(correspondence): Email: gal@dr.lv.ukrtel.net

Intl. Conference on Solid State Crystals 2000: Growth, Characterization, and Applications of Single Crystals, Antoni Rogaski, Krzysztof Adamiec, Pawel Madejczyk, Editors, Proceedings of SPIE Vol. 4412 (2001) © 2001 SPIE · 0277-786X/01/$15.00

3. RESULTS of ELECTRICAL STUDIES

Electrical measurements (current-voltage and capacitance-voltage) were carried out on the monocrystalline samples of the structure In/p-Ag_3SbS_3 (E_g=2.05 eV at 300 K, $\rho \approx 10^5$-10^6 Ω·cm) of electric area A_{el} = 2-5 mm^2. All the studies described below were performed at the room temperature; the investigated samples had not been underwent an additional treatment, In-contacts were prepared by fusion under normal atmospheric conditions.

Figure 2 presents the main results of electric studies.

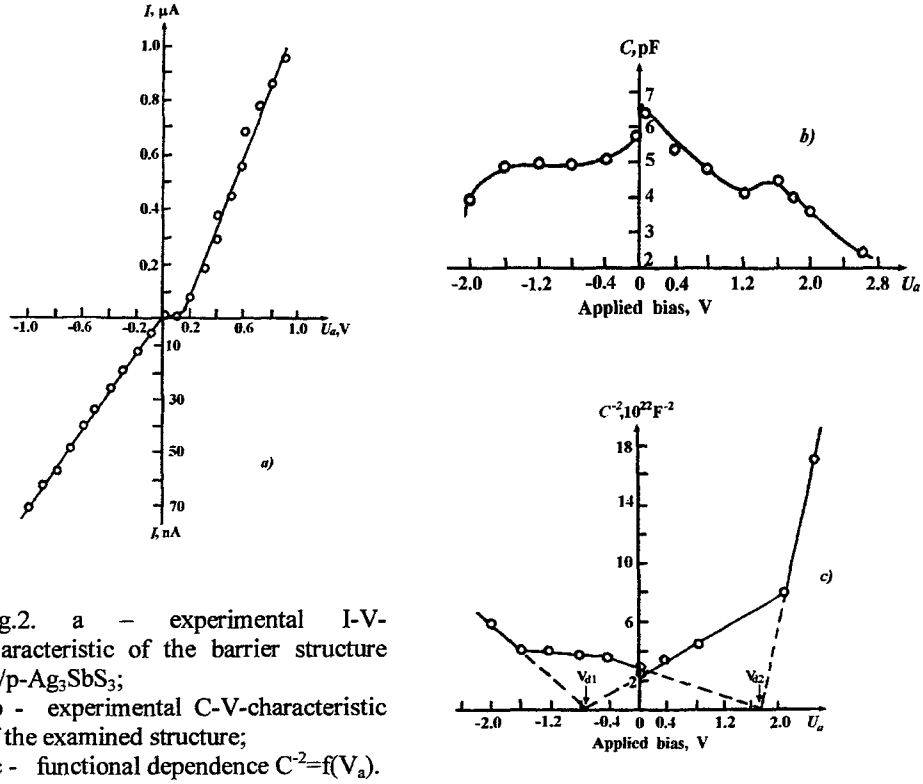

Fig.2. a – experimental I-V-characteristic of the barrier structure In/p-Ag_3SbS_3;
b - experimental C-V-characteristic of the examined structure;
c - functional dependence $C^{-2}=f(V_a)$.

Current-voltage (I-V) characteristics were measured under applied bias V_a = 0÷1 V (Fig.2, a). As one can see, the experimental functional dependence $I(V_a)$ is seemed to be typical for the diode structures: the exponential section (0 ÷1 μA) is qualitatively described by the expression:

$$I = f(m.p., V_a) \exp (eW/nkT), \quad (1)$$

where *f(m.p., V_a)* is a complete function depending on the parameters of Ag_3SbS_3 monocrystals and applied voltage, *W* is an energy parameter (see below), *n* is a non-ideality factor of I-V forward section; the sublinear section (0 ÷ 70 nA) is observed under the opposite direction of applied voltage.

The capacitance-voltage (C-V) dependencies studied under the testing signal frequency *f = 1 kHz* are plotted in Fig. 2, b. It is obvious that the C-V-characteristic of In/p-Ag_3SbS_3 structure is similar to one of the double-saturation barrier structures with graded distribution of impurities in the base. The function $C^{-2} = f(V_a)$ (Fig. 2, c) is linear and demonstrates two barriers 0.8 eV and 1.6 eV in "forward" direction and 0.86 eV and 1.62 eV under reverse bias (the total applied voltage was about 2 V which is closed to the bandgap of Ag_3SbS_3).

More detailed analysis of current-voltage characteristics has showed the availability of complete mechanism of charge carriers transfer.

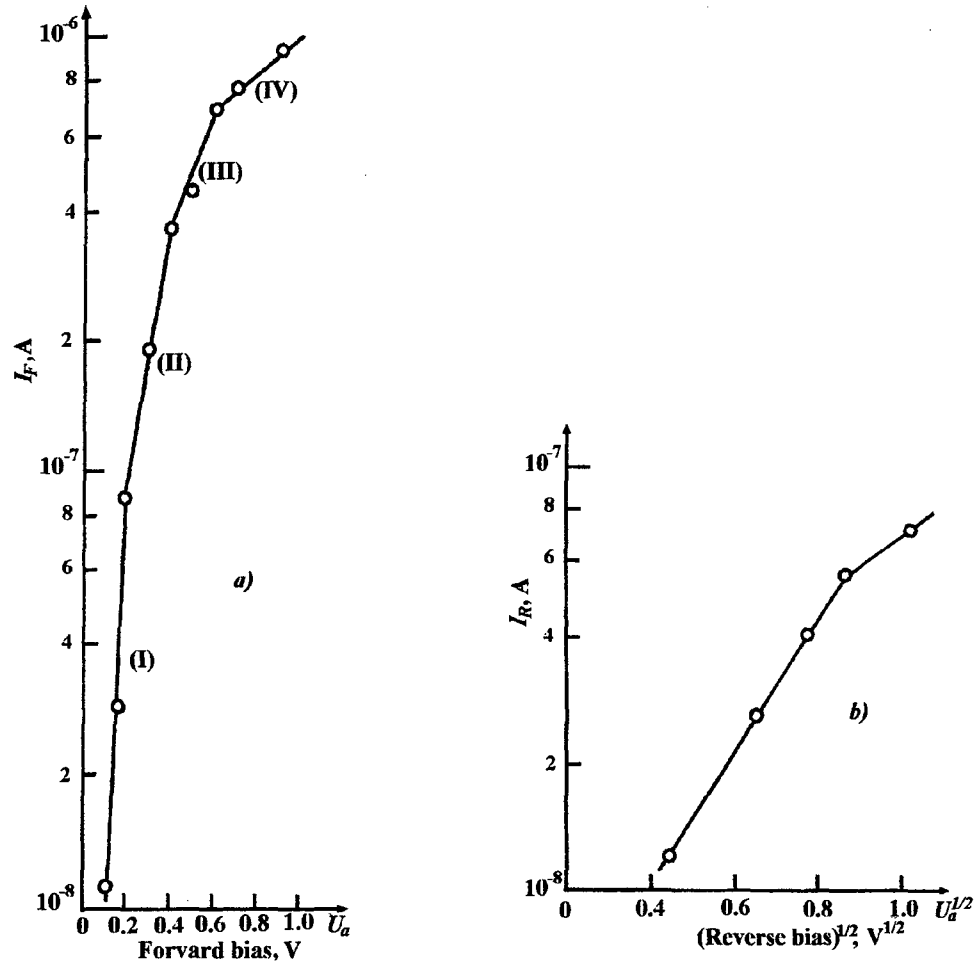

Fig. 3. Semi- (plot *a*) and double- (plot *b*) logarithmic graphs built according to the experimental data.

In particular, the exponential section of the I-V-characteristic (Fig. 3, a) shows tunneling current dominated under applied bias up to 0.6 V (sections I and II, n = 19.1 and 6.3,respectively); as the applied voltage increases up to 0.8 V, charge carriers tunneling changes by tunneling-recombination processes (section III, $n \approx 2.75$) and at Va close to 1 V diffusion process starts to dominate (section IV, $n \approx 0.8$).

Fig. 3, b plots the reverse section of the I-V-characteristic in coordinates $I = f(V_a^{1/2})$ and also shows that tunelling processes are dominant in current transfer at the whole range of applied voltage. The flex point at $V_{TR.rev}$ = 0.84 V (the so-called threshold voltage under the reverse bias) points out the mild break-down indicated an sufficient increase of charge carriers immediately taking part in current transfer.

4. NUMERICAL SIMULATION OF EXPERIMENTAL CURRENT-VOLTAGE CHARACTERISTICS

Numerical modeling of the experimental results is an effective tool of nondestructive monitoring of the studied material properties. In our case such an analysis is performed according to the method described in[2-3] .

Experimental current-voltage characteristics point out the space-charge limited (SCL) current prevalent in the carriers transport in the examined structure. Two modes of the charge carriers transfer are observed experimentally:

$$I = \frac{2\varepsilon_0 \varepsilon v_{sat} A}{L^2} V_a, \tag{2}$$

under the applied bias > 0.7 V, in the range of applied voltage from 0 to 0.6 V the expression described the current is given below:

$$I = \frac{9\varepsilon_0 \varepsilon A \mu V_a^2}{8L^3}, \tag{3}$$

and the reverse section of the experimental I-V-characteristic is presented by the equation of ballistic mode of majority charge carriers transport:

$$I = \frac{4\varepsilon_0 \varepsilon A}{9L^2}\left(\frac{2e}{m_h^*}\right)^{1/2} V_a^{3/2}, \tag{4}$$

where A, L, V_a, v_{sat}, μ are the sample area, its length, apllied bias,saturation velosity (expession (4) produced by the solution of eqs (1) and (3)) and the charge carriers mobility, respectively.

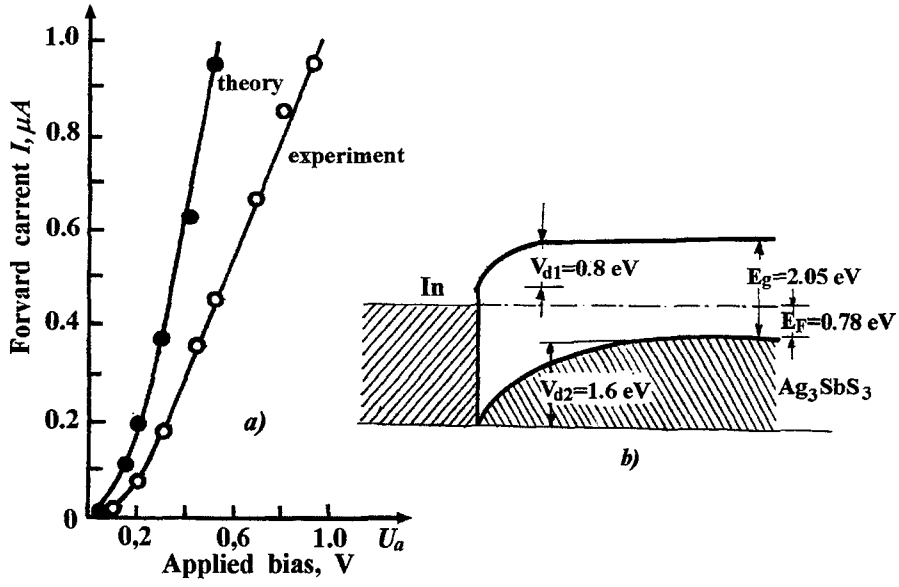

Fig. 4. a – numerically simulated and experimental forward current-voltage characteristics of the barrier structure In/p-Ag_3SbS_3; b- static energy band diagram. T=290 K.

$$v_{sat} = \sqrt{\frac{8eV_{TR}}{81m_h^*}}. \quad (5)$$

Numerical simulation was carried out for the forward I-V-dependence because the peculiarities of the crystallographic structure of Ag_3SbS_3 indicates on considerable effect of intrinsic intercrystalline barriers. The reverce current-voltage dependence is influenced not only by the precesses described above, but also by silver oxide formed on the pyrargyrite monocrystal surface revealed by Ag_3SbS_3 Auger-profiling of elemental composition[4].

The modeled forward current-voltage characteristic (5) considering the majority charge cariers tunneling in the monocrystal bulk is shown in Fig. 4, a. Here d is a distance between ajoined chains ...-S –Ag – S... in Ag_3SbS_3 monocrystal, m_h^* is holes effective mass, V_d is difussion potential determined by the capacitance-voltage measurements.

$$I_{ther} = \left(\frac{2\varepsilon_0\varepsilon v_{sat} A}{l^2}V_a + \frac{9\varepsilon_0\varepsilon A\mu}{8L^3}V_a^2\right)\exp\left(\frac{-4d(2m_h^*)^{1/2}}{3\hbar}\right)\exp\left(\frac{-E_g}{kT}\right)\exp\left(\frac{V_a - V_d}{nkT}\right) \quad (6)$$

A good agreement is observed in the range of voltage 0 – 150 mV and a quantity coincidence is shown as the applied voltage increases. The discrepancy of simulated and experimental results can be explained by the additional influence of leakage current and the minority charge carriers tunneling in the subcontact region and surface oxide layer.

5. CONCLUSIONS

Electric investigations of metal-semiconductor structure based on monocrystal p-Ag_3SbS_3 carried out at the room temperature were shown barrier characteristics typical for the double saturation diode-like structures. The space-charge limited (SCL) current is observed in the whole range of applied voltage. The results obtained experimentally indicate that the electrical behavior of the examined structure is influenced by the peculiarities of the crystallographic structure of Ag_3SbS_3 monocrystals as well as by the AgO layer formed on Ag_3SbS_3 surface.

REFERENCES

1. P. Engel and W. Nowacki, "Die Verfeinerung der Kristallstruktur von Proustite (Ag_3AsS_3) and Pyrargyrite (Ag_3SbS_3)", *Neues Jahrb. Mineralogie*, No.6, pp.191-195, 1966.
2. E. Hernandez, "Space-Charged-Limited Current Effects in p-Type $CuIn_{0/8}Ga_{0.2}Se_2$/In Schottky Barriers", *Cryst. Res. Technol.*, 33, pp.285-289, 1998.
3. N. G. Kwok, *"Complete Guide to Semiconductor Devices"*, pp. 564-565, McGrow Hill, New York, 1995.
4. V. Belosertseva, V. Basakutsa and L. Panchenko, "Structure and Crystallization of Ag_3SbS_3 layers obtained by Pulse Laser Evaporation", *Cryst. Res. Technol.*, 34, pp. 677-682, 1999.