



# Forward and reverse bias current–voltage ( $I$ – $V$ ) characteristics in the metal–ferroelectric–semiconductor ( $\text{Au}/\text{SrTiO}_3/\text{n-Si}$ ) structures at room temperature

A. Buyukbas-Ulusan<sup>1</sup> · S. Altındal-Yerişkin<sup>2</sup> · A. Tataroğlu<sup>1</sup>

Received: 27 April 2018 / Accepted: 27 July 2018 / Published online: 31 July 2018  
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## Abstract

The main electrical parameters of fabricated  $\text{Au}/\text{SrTiO}_3/\text{n-Si}$  (MFS) structures have been investigated by using various methods. The values of ideality factor ( $n$ ) and zero-bias barrier height ( $\Phi_{B0}$ ) are calculated from the forward bias current–voltage ( $I_F$ – $V_F$ ) data as 0.60, and 0.48 eV from thermionic theory (TE) and Cheung functions, respectively. The value of  $R_s$  is also obtained from the Norde function and Cheung functions as 87.83 and 137.57  $\Omega$ , respectively. The discrepancy between these results can be attributed to the calculated method and the measured voltage range. Besides, the energy density distribution profile of interface state ( $N_{ss}$ ) was obtained from the ( $I_F$ – $V_F$ ) data by taking into account voltage dependent barrier height (BH),  $n$  and without  $R_s$ . On the other hand, the possible current conduction mechanism (CCM) are determined by utilizing the  $\ln(I_F)$  versus  $\ln(V_F)$  and  $\ln(I_R)$  versus  $V_R^{1/2}$  plots. The double logarithmic  $I_F$ – $V_F$  plot shows three linear regions which are corresponding to low, moderate and high bias voltages with different slopes ( $m$ ) as 2.40, 1.96 and 1.27 respectively. While the first region space charge limited current (SCLC) is dominated, the other two regions ohmic behavior is dominated. The field-lowering coefficient ( $\beta$ ) was also obtained from the slope of  $\ln(I_R)$ – $V^{1/2}$  plot as  $4.40 \times 10^{-6} \text{ eV}^{-1} \text{ m}^{1/2} \text{ V}^{1/2}$ . This value of  $\beta$  is close to theoretical value of Poole–Frenkel emission (PFE) rather than Schottky emission (SE) mechanism.

## 1 Introduction

Strontium-titanate-oxide (STO) has  $\text{SrTiO}_3$  chemical formula and some important properties such as a high charge storage capacity, wide bandgap (3.25–3.95 eV), high dielectric constant ( $\epsilon = 310$ ) excellent optical transparency in the visible region and chemical stability [1, 2]. Therefore, it has been used in microelectronic materials and semiconductor devices such as tunable high temperature superconducting microwave filters, metal–insulator/oxide semiconductor (MIS and MOS), metal–polymer–semiconductor (MPS), MOS field-effect transistors (MOSFETs), ultra-low-temperature scanning microscopes, oxygen sensors, magnetic field insensitive thermometer etc [1–6]. STO film can be also fabricated by various methods such as radio frequency

(RF) magnetron sputtering, metal–organic chemical vapor deposition (MOCVD), molecular beam epitaxy (MBE), and sol–gel and it crystallizes in the  $\text{ABO}_3$  cubic perovskite structure at room temperature. However, for temperature less than 105 K, it returns to the tetragonal structure [4]. Therefore, in this study, STO was used as interfacial layer between metal and semiconductor to improve the quality or performance of  $\text{Au}/\text{n-Si}$  (MS) structure.

The forward and reverse bias  $I$ – $V$  measurements can be supplied more information on the main electrical parameters and possible the CCMs. The main electrical parameters such as the  $n$ , reverse saturation current ( $I_0$ ),  $\Phi_{B0}$  and energy–density distribution of  $N_{ss}$  can be calculated by using the thermionic emission (TE) theory. But, both the existence of  $R_s$ , high-dielectric interfacial layer and  $N_{ss}$  are more effective on the CCMs. Because, the applied voltage across the diode/structure will be shared by them. Therefore, value of  $R_s$  was obtained from both the Norde and Cheung’s functions. On the other hand, the reverse bias  $I_R$ – $V_R$  plot can be supplied on CTMS [7–12]. For instance, at forward bias region, the space charge limited current (SCLC), trap charge limited current (TCLC) or ohmic behavior can be dominated in the CCMs. When the electrons injections are high and electrons

✉ A. Buyukbas-Ulusan  
aysel.buyukbas@gmail.com

<sup>1</sup> Physics Department, Faculty of Sciences, Gazi University, Ankara, Turkey

<sup>2</sup> Department of Chemical Engineering, Faculty of Engineering, Gazi University, Ankara, Turkey

escape from the traps, the SCLC mechanism can occur. But, the filling of traps and increase of the space charge because of the number of injected electrons increase can be occurred at the TCLC mechanism [6, 13]. On the other hand, at the reverse bias regions, the Schottky (SE) or Poole–Frenkel (PF) emission may be dominated in the CCMs. According to the SE, current transport occurs across the contact interface instead of the bulk material, but based on the Poole–Frenkel emission, the current transport occurs from the metal into conductive dislocations via trap states [6, 14].

The grown of high-dielectric interfacial layer between metal and semiconductor interface is more importance to the performance and reliability of the MS structures. Therefore, in recently, high-dielectric materials such as  $\text{TiO}_2$ ,  $\text{SrTiO}_3$  (STO),  $\text{Bi}_4\text{Ti}_3\text{O}_{12}$  (BTO) and graphene-doped PVA take the place of the traditional  $\text{SiO}_2$  and  $\text{SnO}_2$ . It is believed that the traditional  $\text{SiO}_2$  formed on a semiconductor by the traditional methods cannot passivate the active dangling bonds at the semiconductor surface. On the other hand, this high-dielectric material can be reduced the active dangling bonds and so leads to a decrease of the leakage current, surface states, series resistance and increased of BH. However, the use of a high dielectric interfacial layer does not only prevent inter-diffusion at M/S interface but also alleviates the electric field reduction issue in these structures [15–18]. Therefore, in this study,  $\text{SrTiO}_3$  was used an interfacial ferroelectric layer between Au and n-Si.

The main aim of this study is characterization of the electrical properties of Au/n-Si structure with high-dielectric  $\text{SrTiO}_3$  interfacial ferro-electric layer by utilizing both reverse and forward bias current–voltage (I–V) measurements in the wide range of voltage ( $\pm 5$  V) at room temperature. Main electrical parameters of this MFS type structure such as  $n$ ,  $\Phi_{B0}$ ,  $R_s$  were obtained by using various methods (TE, Norde and Cheung's). The energy dependent profile of  $N_{ss}$  was calculated for from the forward bias  $I_F$ – $V_F$  data by taking into account voltage dependent BH,  $n$ , and  $R_s$ . The possible CCMs were also determined from both the reverse and forward bias region.

## 2 Experimental details

Au/ $\text{SrTiO}_3$ /n-Si structure was prepared on n-Si wafer which has (111) surface orientation, 280  $\mu\text{m}$  thick, 5.08 cm diameter and 4.45  $\Omega$  cm resistivity. Firstly, the n-Si wafer cleaning and etching processes is traditionally done by using different chemical solvent in ultrasonic bath and then it was rinsed using deionized water with 18  $\Omega$  cm resistivity and finally dried with dry nitrogen gas ( $\text{N}_2$ ). After the cleaning process, the wafer was heated optically and loaded into a radio frequency (RF) magnetron sputtering system. The  $\text{SrTiO}_3$  (STO) thin film was deposited by RF magnetron sputtering

method on n-Si wafer. Then, the film was heated at 400  $^\circ\text{C}$  in air for 30 min to remove residual organic. High purity (99.999%) gold (Au) with a thickness of  $\sim 2000$   $\text{\AA}$  was deposited on the whole back side of the n-Si wafer at  $10^{-7}$  Torr by using the high-vacuum metal evaporation system through a shadow Cu mask. In order to get low resistivity ohmic back contact, STO/n-Si wafer was annealed at 700  $^\circ\text{C}$  for 60 min in flowing nitrogen ambient at rate of 2 L/min. Finally, the wafer was placed in the same evaporation system and then the high-pure Au rectifier contact with 1 mm diameter and approximately 2000  $\text{\AA}$  thick formed on the front of n-Si wafer at a rate of 4  $\text{\AA}/\text{s}$  through a Cu shadow mask. Thus, the fabrication processes of Au/ $\text{SrTiO}_3$ /n-Si (MFS) type structures were completed. For the electrical measurements, the fabricated samples were placed on the copper holder and the contacts were made by silver paste and the electrical contacts were also made to the upper electrodes using small thin silver coated wires with silver paste. The current–voltage (I–V) measurements of the structure were carried out with utilizing Keithley 2400 source meter in the VPF-475 cryostat to avoid an external noise and light at room temperature. The sample temperature was monitored by using a copper–constantan thermocouple and a lakeshore 321 auto-tuning temperature controller with sensitivity better than  $\pm 0.1$  K.

The schematic diagram of the fabricated Au/ $\text{SrTiO}_3$ /n-Si (MFS) type structures and the measurement forward and reverse bias I–V measurements were given in Fig. 1.

## 3 Results and discussion

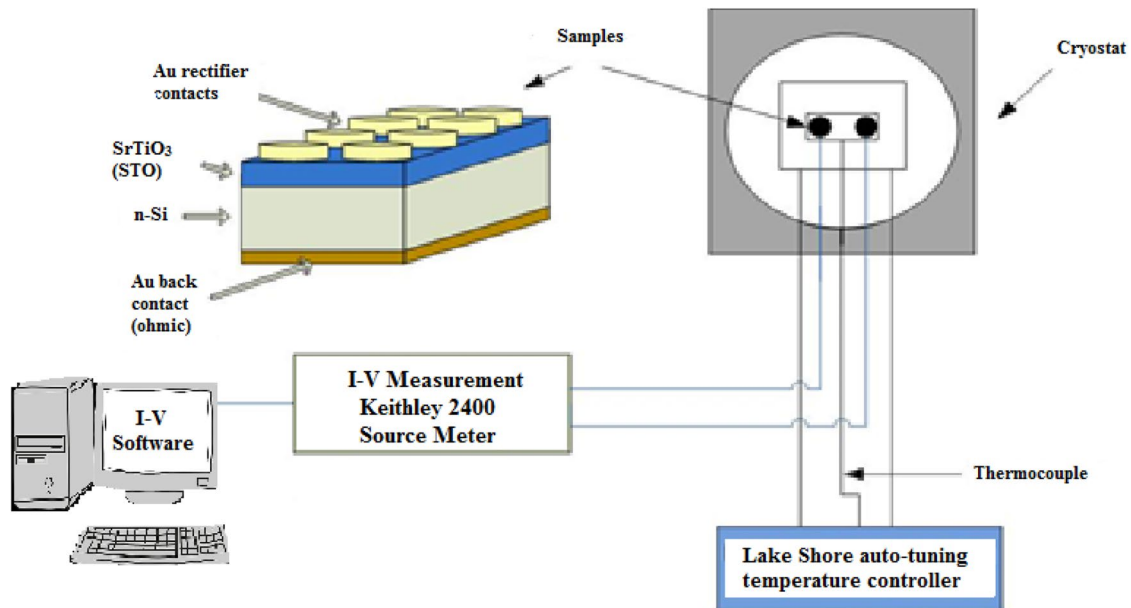
The conduction mechanism of a diode is defined by utilizing the thermionic emission (TE) theory. According to this theory, the forward bias I–V relation can be expressed as [6];

$$I = I_0 \left[ \exp \left( \frac{q(V - IR_s)}{nkT} \right) - 1 \right] \quad (1)$$

where  $I_0$  is the reverse saturation current,  $V$  is applied bias voltage,  $q$  is the electric charge ( $1.6 \times 10^{-19}$  coulombs),  $k$  is the Boltzmann constant ( $1.38 \times 10^{-23}$  J/K),  $n$  is the ideality factor,  $T$  is the absolute temperature (K),  $R_s$  is the series resistance of the sample and the  $IR_s$  term is voltage drop on  $R_s$ . The  $I_0$  is given by following equation for any temperature;

$$I_0 = AA^*T^2 \exp \left( -\frac{q\Phi_{B0}}{kT} \right) \quad (2)$$

where  $A$  is the rectifier contact area ( $7.85 \times 10^{-3}$   $\text{cm}^2$ ),  $A^*$  is the effective Richardson constant (112 for n-Si),  $\Phi_{B0}$  is the zero bias barrier height. Firstly, the value of  $I_0$  can be



**Fig. 1** The schematic diagram of the fabricated Au/SrTiO<sub>3</sub>/n-Si (MFS) type structures and the I–V measurement system

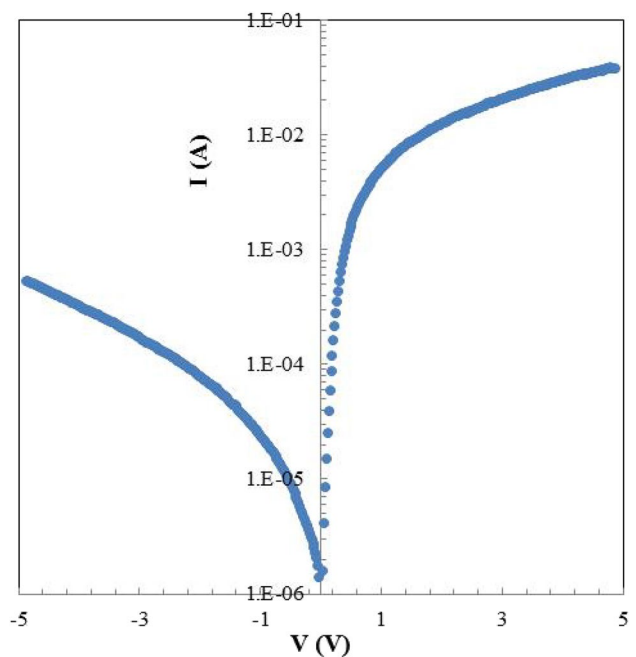
obtained from the intercept of the linear part of the forward bias current–voltage characteristic and then the  $\Phi_{B0}$  is defined by following equation:

$$\phi_{B0} = \frac{kT}{q} \ln \left( \frac{AA^*T^2}{I_0} \right) \quad (3)$$

The ideality factor ( $n$ ) of the diode is obtained by using the experimental forward bias current–voltage data. It was calculated from the slope of the linear part of the forward bias current–voltage characteristic and may be written as

$$n = \frac{q}{kT} \left( \frac{dV}{d(\ln I)} \right) \quad (4)$$

The reverse and forward bias semi-logarithmic I–V plot of the Au/SrTiO<sub>3</sub>/n-Si (MFS) structure is illustrated in Fig. 2. As shown in Fig. 2, the forward bias current plot in the range of  $0.1 \text{ V} < V < 0.3 \text{ V}$  shows a distinct linear behavior and then because of the effect  $R_s$  and interlayer the semi-logarithmic I–V plot is deviated from the linearity. Since the voltage applied on the sample it will be shared by depletion layer, interfacial layer and  $R_s$ . But the effect of  $R_s$  can be eliminated low in the linear part of  $\ln I$ –V plot [19, 20]. The non-saturation behavior in the reverse current can be commonly explained in the terms of the image force lowering of the BH between metal and semiconductor and inhomogeneity of barrier height. If we used this linear part, we can calculate the values of both  $\Phi_{B0}$  and  $n$ . The values of  $\Phi_{B0}$  and  $n$  are found as 0.60 eV and 2.45 by using the TE at room temperature, respectively. Similar result have been reported



**Fig. 2** The semi-logarithmic forward and reverse I–V characteristic of the Au/SrTiO<sub>3</sub>/n-Si (MFS) structure at room temperature

in the literature for MIS [19–23], MPS [24] and MFS [18] structures.

As can be seen in Fig. 2, the value of  $R_s$  is more effective on the forward bias I–V characteristics and leads to deviated from the linearity of I–V plot at enough high forward bias voltage. In general,  $R_s$  can originate from five different sources; (a) the back ohmic contact to the semiconductor,

(b) the contact made by the probe wire to the gate or rectifier contact, (c) the bulk resistance of the semiconductor, (d) a particulate matter at back contact/pedestal interface and (e) non-uniform doped atoms in the semiconductor [23, 25]. It can be reduced either by having a low BH at M/S interface or by having an enhanced tunneling through the barrier by using heavy doped semiconductors ( $\geq 10^{17} \text{ cm}^{-3}$ ) or by the use of a good cleaning and fabrication process. In order to the estimation of the  $R_s$  from the forward bias I–V data one of the most commonly used methods are the modified Norde functions by Bohlin [26] and Cheung [27] functions. According to Bohlin, an alternative easy method to determine the barrier height ( $\Phi_B$ ) and  $R_s$  can be expressed as [26]:

$$F(V) = \frac{V}{\gamma} - \frac{kT}{q} \left[ \ln \left( \frac{I(V)}{AA^*T^2} \right) \right] \tag{5}$$

where  $\gamma$  is a dimensionless integer and it should be selected greater than  $n$ . According to this method, the values of  $\Phi_B$  and are given by Eqs. 6 and 7, respectively.

$$\Phi_B = F(V_o) + \frac{V_o}{\gamma} - \frac{kT}{q} \tag{6}$$

where  $F(V_o)$  is the minimum value of the  $F(V)$ – $V$  plot. Thus the value of  $R_s$  can be extracted from the Norde function as:

$$R_s = \frac{kT(\gamma - n)}{qI_{\min}} \tag{7}$$

The  $F(V)$  versus  $V(V)$  plot of Au/SrTiO<sub>3</sub>/n-Si (MFS) structure at room temperature is given in Fig. 3. This plot gives a minimum point and both  $\Phi_B$  and  $R_s$  are calculated by utilizing this minimum point. The values of  $\Phi_B$  and  $R_s$  were found 0.61 eV and 87.83  $\Omega$  at room temperature, respectively.

Also, the values of  $R_s$ ,  $n$  and  $\Phi_B$  can be obtained from another alternative method which is known as Cheung functions. Cheung’s functions were defined as [27];

$$\frac{dV}{d(\ln I)} = IR_s + \left( \frac{nkT}{q} \right) \tag{8}$$

and

$$H(I) = V - \frac{nkT}{a} \ln \left( \frac{I}{AA^*T^2} \right) = IR_s + n\phi_{B0} \tag{9}$$

Both the  $dV/d(\ln I)$  versus  $I$  and  $H(I)$  versus  $I$  plots are illustrated in Fig. 4. It is clear that these two plots have a good linear behavior in the wide range of forward bias current. The value of  $R_s$  is found from the slope of the both  $dV/d(\ln I)$  versus  $I$  and  $H(I)$  versus  $I$  plots. The obtained  $R_s$  values from these slopes are found as 137.57 and 121.04  $\Omega$ , respectively. It is shown that, the calculated values of  $R_s$  are in close agreement with each other. On the other hand, the value of  $n$  was found as 2.95 from the intercept of  $dV/d(\ln I)$  versus  $I$  plot. After that, the value of  $\Phi_B$  was obtained

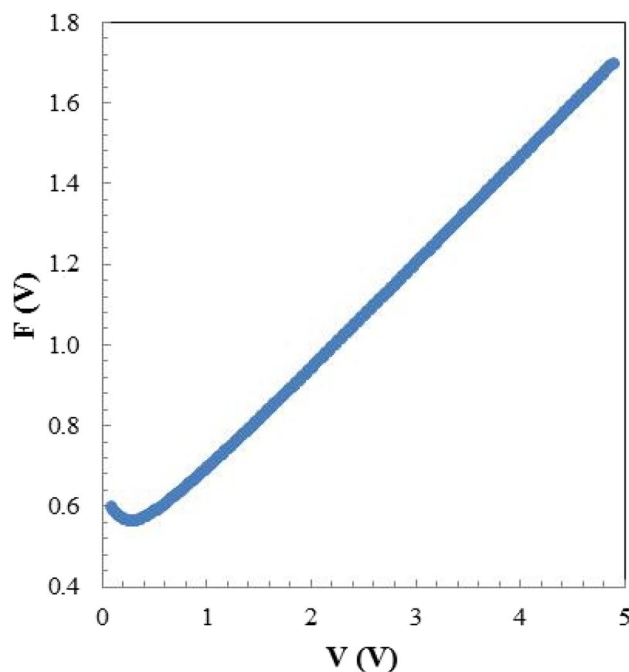


Fig. 3  $F(V)$  versus  $V (V)$  plot of the Au/SrTiO<sub>3</sub>/n-Si (MFS) structure at room temperature

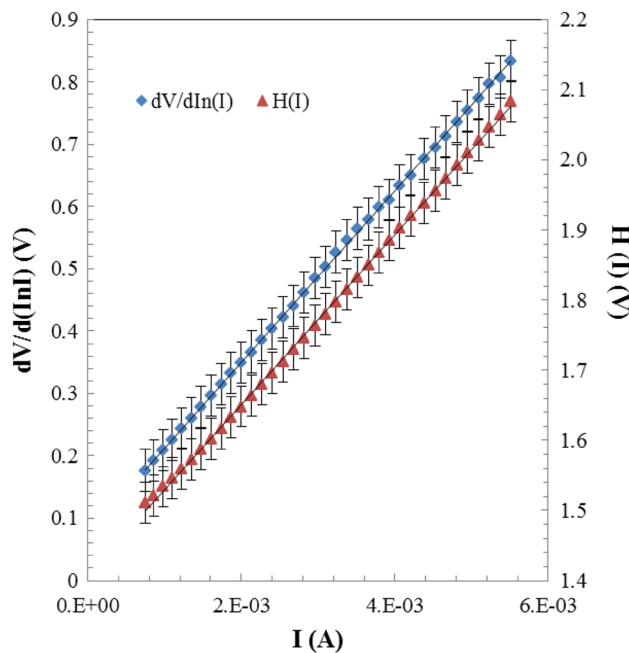


Fig. 4  $dV/d(\ln I)$  and  $H(I)$  versus  $I$  plots of Au/SrTiO<sub>3</sub>/n-Si (MFS) structure at room temperature

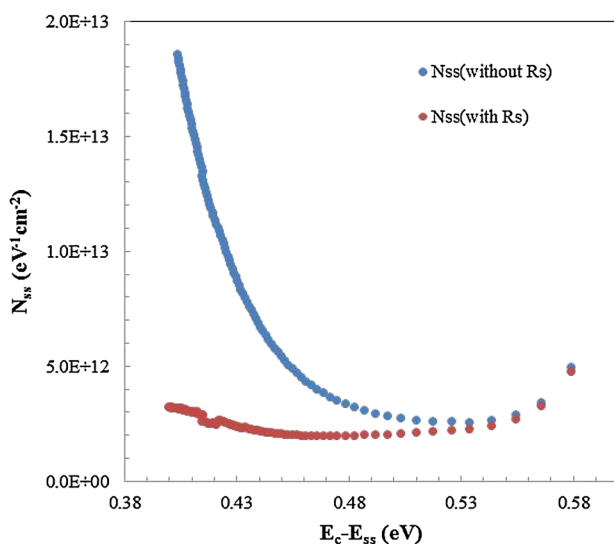
as 0.48 eV from the intercept of  $H(I)$  versus  $I$  plot. This discrepancy in  $n$  and  $\Phi_B$  is the result of voltage dependent [6, 7].

The existence of  $N_{ss}$  located between interfacial layer and semiconductor are also more effective on the forward bias I–V characteristics. Unless specifically manufactured the MS, MIS, MPS and MFS structures, many  $N_{ss}$ , bulk traps and dislocations can be occurred which lead to electronic states with energies located in the forbidden band gap of the semiconductor between metal and semiconductor. When the interfacial layer thickness is higher than 30 Å, these states/traps are equilibrium with semiconductor rather than metal. These states can be altered the performance of these devices and they usually originated from defects such as dangling bounds at the insulator/substrate interface with energy states in the semiconductor band gap ( $E_g$ ) and are dependent on the chemical composition of the interface [6, 7, 22, 27]. Therefore, the density of  $N_{ss}$  for the Au/SrTiO<sub>3</sub>/n-Si (MFS) structure was also calculated by using following equations (Eqs. 10–13) by taking into account voltage dependent effective BH ( $\Phi_e$ ),  $n(V)$  and  $R_s$  and presented in Fig. 5 [7, 22, 27]:

$$N_{ss}(V) = \frac{1}{q} \left[ \frac{\delta}{\epsilon_i} (n(V) - 1) - \frac{\epsilon_s}{W_D} \right] \quad (10)$$

where,  $\delta$  is the thickness of interfacial insulator layer ( $5 \times 10^{-7}$  cm),  $W_D$  is the depletion layer width,  $\epsilon_i$  is permittivity of the interfacial insulator layer,  $\epsilon_s$  is permittivity of the semiconductor and  $\epsilon_0$  is the permittivity of the free space.

$$n(V) = \frac{qV_d}{kTLn(I/I_0)} \quad (11)$$



**Fig. 5**  $N_{ss}$  versus  $E_c - E_{ss}$  plots with and without of  $R_s$  for the Au/SrTiO<sub>3</sub>/n-Si (MFS) structure at room temperature

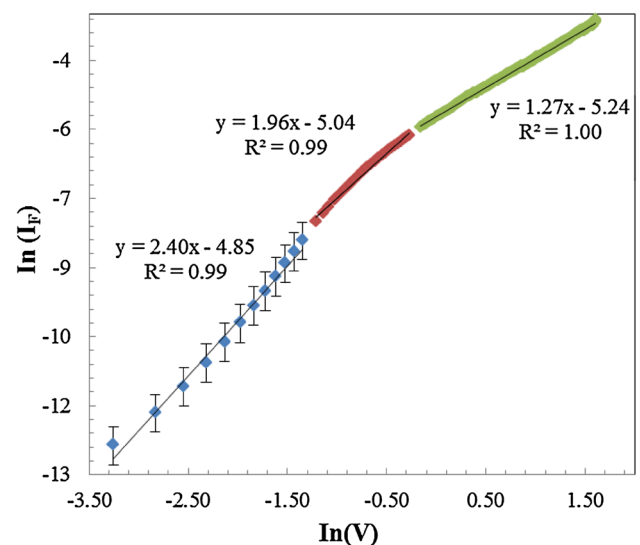
Moreover, the energy dependent value of the  $N_{ss}$  with respect to the top of the conduction band ( $E_c$ ) at the surface of semiconductor is given as:

$$E_c - E_{ss} = q(\Phi_e - V_d) \quad (12)$$

$$\Phi_e - \Phi_{B0} = \left(1 - \frac{1}{n(V)}\right) V_d \quad (13)$$

In Eqs. 1–13,  $V_d$  is the voltage across on the structure ( $= V - IR_s$ ). When these structures have an interfacial layer and  $R_s$ , the applied bias voltage will be shared by them. The calculated mean value of  $N_{ss}$  is approximately  $10^{13} \text{ eV}^{-1} \text{ cm}^{-2}$  and this value may be noted suitable for a semiconductor device. However, these values with  $R_s$  is almost one order lower than the without  $R_s$ . All of these results show that both the value of  $R_s$  and interfacial layer thickness must be taken into account in the calculations.

In order to determine separately the dominant current transport mechanisms in both the forward and reverse bias regions,  $\ln(I_F)$  versus  $\ln(V)$  and  $\ln(I_R)$  versus  $V^{1/2}$  plots were drawn. The first of these is the  $\ln(I_F)$  versus  $\ln(V)$  plot and is shown in Fig. 6. This plot has three distinct linear regions which have different slopes. The region 1 ( $-3.25 < V < -1.35$ ), region 2 ( $-1.21 < V < -0.28$ ) and region 3 ( $-0.15 < V < 1.61$ ) obey I– $V^m$  change. The  $m$  is the slope of each region and was obtained 2.40, 1.96 and 1.27 respectively. At first region which is known as low bias region, the dominant conduction mechanism is space charge limited current (SCLC) because of the value of  $m$  is higher than two. On the other hand at second region which is known as moderate bias region and third region which is known as high bias region, the dominant conduction mechanism



**Fig. 6** The  $\ln(I_F)$  versus  $\ln(V)$  plot of the Au/SrTiO<sub>3</sub>/n-Si (MFS) structure at room temperature



is ohmic behavior because of the value of  $m$  is close to the unity [28–32]. The obtained experimental main electrical parameters of the Au/SrTiO<sub>3</sub>/n-Si (MFS) structure show that the possible current conduction mechanism in the forward bias region may be different from region to region depend on a special distribution of  $N_{ss}$ , barrier and interfacial layer inhomogeneity between metal and semiconductor.

The reverse bias I–V characteristics is general different from the forward bias I–V characteristics. In the reverse bias region, the current mechanisms are usually can be explained by using Poole–Frenkel emission (PFE) and Schottky emission (SE) theories. If the PFE mechanism is dominant, the reverse current can be expressed as [14, 29–35]:

$$I_R = I_0 \exp\left(\frac{\beta_{PF} V^{1/2}}{kT d^{1/2}}\right) \tag{14}$$

If the SE mechanism is dominant, the reverse current can be expressed as;

$$I_R = AA^* T^2 \exp\left(\frac{-\Phi_b}{kT}\right) \exp\left(\frac{\beta_{SC} V^{1/2}}{kT d^{1/2}}\right) \tag{15}$$

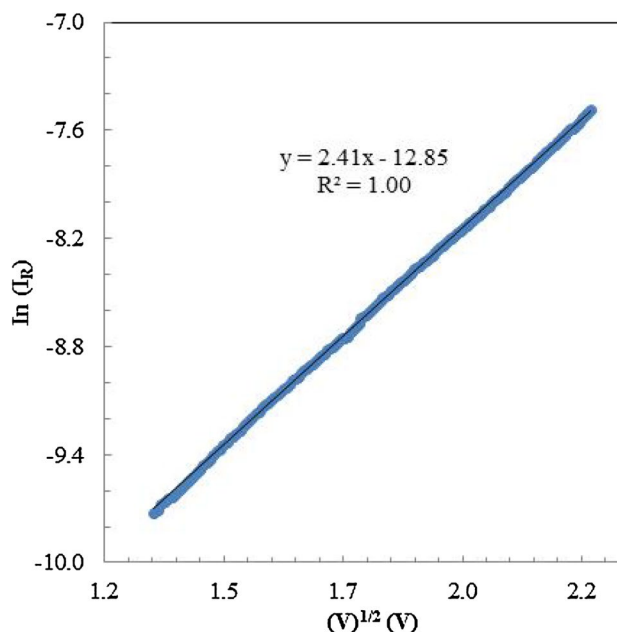
where  $\beta_{PF}$  and  $\beta_{SC}$  are the field-lowering coefficients of PFE and SE, respectively. The theoretical values of these coefficients are given in following equation.

$$2\beta_{SC} = \beta_{PF} = \left(\frac{q^3}{\pi\epsilon_0\epsilon_r}\right)^{1/2} \tag{16}$$

where  $\epsilon_r$  is the relative permittivity of interfacial layer. As shown in Eq. 16, the value of  $\beta_{PF}$  is always twice the value of  $\beta_{SC}$ . The theoretical value of both  $\beta_{PF}$  and  $\beta_{SC}$  are found as  $4.30 \times 10^{-6}$  and  $2.1 \times 10^{-6} \text{ eV}^{-1} \text{ m}^{1/2} \text{ V}^{1/2}$ , respectively. The  $\ln(I_R)$  versus  $V^{1/2}$  plot of Au/SrTiO<sub>3</sub>/n-Si structure is shown in Fig. 7. As seen in Fig. 7, the plot has a district linear variation. The field-lowering coefficient is found by using of the slope of this linear region. The value of field-lowering coefficient is calculated as  $4.40 \times 10^{-6} \text{ eV}^{-1} \text{ m}^{1/2} \text{ V}^{1/2}$ . The obtained value of field-lowering coefficient is close to theoretical value of PFE coefficient. This result shows that the dominant reverse bias conduction mechanism is PFE mechanism. So, the carrier transport is formed from the metal into conductive dislocations via trap states.

### 4 Conclusions

In this study, both the reverse and forward bias current–voltage (I–V) characteristics in the Au/SrTiO<sub>3</sub>/n-Si (MFS) structure have been analyzed in the wide range of voltage ( $\pm 5 \text{ V}$ ) at room temperature by using various methods. The value of  $\Phi_{B0}$  is found as 0.60, 0.61 and



**Fig. 7**  $\ln(I_R)$  versus  $V_R^{1/2}$  plot of the Au/SrTiO<sub>3</sub>/n-Si (MFS) structure at room temperature

0.48 eV by using the TE, Norde function and Cheung functions, respectively. The value of  $n$  is found as 2.45 and 2.95 by using the TE and Cheung functions, respectively. The value of  $R_s$  was found as 87.83  $\Omega$  (from Norde function), 135.87  $\Omega$  [from  $dV/d\ln(I)$  vs.  $I$  plot] and 121.04  $\Omega$  [from  $H(I)$  vs.  $I$  plot]. The energy density distribution of  $N_{ss}$  for the MFS structure was obtained from the forward-bias I–V data by taking into account voltage dependent  $\Phi_e$ ,  $n$  and  $R_s$ . The calculated value of the  $N_{ss}$  is  $\sim 10^{13} \text{ eV}^{-1} \text{ cm}^{-2}$  without of  $R_s$  but they found as  $\sim 10^{12} \text{ eV}^{-1} \text{ cm}^{-2}$ . In addition, the possible dominant current transport mechanisms of both forward and reverse bias regions were determined by using the  $\ln(I_F)$  versus  $\ln(V)$  and  $\ln(I_R)$  versus  $V^{1/2}$  plots. The dominant conduction mechanisms of the forward bias regions are SCLC at low bias region and ohmic behavior at high bias region. The obtained results show that the possible current conduction mechanism in the forward bias region may be different from region to region depend on a special distribution of  $N_{ss}$ , barrier and interfacial layer inhomogeneity between metal and semiconductor. The value of field-lowering coefficient is calculated as  $4.40 \times 10^{-6} \text{ eV}^{-1} \text{ m}^{1/2} \text{ V}^{1/2}$  from the reverse bias I–V characteristics and it is close to theoretical value of PFE coefficient. This result shows that the dominant reverse bias conduction mechanism is PFE mechanism. So, the carrier transport is formed from the metal into conductive dislocations via trap states.

**Acknowledgements** This study was supported by Gazi University Scientific Research Project (Project Number: GU-BAP.05/2018-10).

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