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Dominant conduction mechanism and the effects of device temperature on electrical characteristics of Al/ZnPc/n-Si structures

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ABSTRACT

Aluminum/Zinc Phthalocyanine/n-Si metal semiconductor contact with organic interfacial layer has been developed and characterized by Current–Voltage–Temperature (*I–V–T*) measurements for the study of its junction and charge transport properties. The junction parameters, such as diode ideality factor (n), barrier height (φ_b) and series resistance (R_S), of the device were found to shift with device temperature. The diode ideality factor was found to increase with the device temperature up to 323 K. However, a decreasing trend in the value of n was observed beyond this temperature. The barrier height and series resistance were found to increase and decrease, respectively with increasing device temperature. The peak of interface state energy distribution curves was shifted, in terms of Ess-Ev value, from 0.622 eV to 0.827 eV with 52 meV activation energy of the charge carriers. The data analysis implies that the Fermi level of the organic interfacial layer shifts as function of device temperature. In terms of dominant conduction mechanism, the *I–V–T* data analysis confirms the relationship $\log(IV^4) \propto V^{1/2}$ with the device temperature in the range of 313–343 K and the Poole–Frenkel type is found to be the dominant conduction mechanism for the hybrid device.

1. Introduction

The freedom of choice of materials for manufacturing inexpensive lightweight electronic devices based on organic semiconductors and through away molecular electronics on thin and flexible substrates has opened a highly potential area of research for future investigations. The stability of organic compounds is another feature of the materials making them potential candidates to be employed in electronic devices. Electrical properties of molecule/metal and molecule/semiconductor interfaces have been extensively studied in recent years [1–5] to understand the charge transfer properties of the organic/inorganic interfaces. The organic semiconductors are often studied as interfacial layers in metal/semiconductor structures, in terms of n, φ_B and R_S values, as these semiconductors can structurally be modified to engineer the rectification properties of metal/semiconductor contacts [6–10]. These modified Schottky diodes, based on organic/inorganic interfaces, find their potentials technological applications in a number of electronic devices as in nuclear detectors [11,12], organic thin film transistors [13–16] and gas sensors [17].

Dominant conduction mechanism in organic thin films and the organic/inorganic semiconductor interfaces has been extensively reported in recent papers [18–23]. These reports suggest different dominant conduction mechanisms in the respective organic/inorganic structures, which include space charge limited current [18–20], multi step tunneling recombination current [21], Poole–Frenkel conduction [22] and Schottky conduction mechanism [23]. Similarly, in terms of n, φ_B and R_S, different values for the electronic parameters of these organic/inorganic heterojunctions of similar structures have been reported [24]. The present paper reports on the formation of Al/Zinc Phthalocyanine/N-Silicon/AuSb (1%) hybrid structure and subsequent characterization of the structures for investigation of charge transport properties. The hybrid structure behaves differently at different device temperatures. The n, φ_B and R_S values are estimated in the temperature range of 283–343 K. The estimated values were crosschecked by reproducing the respective *I–V* curves at all device temperatures, by adopting the calculated n, φ_B and R_S values in the standard diode equation. Activation energy of charge carries, interface state energy distribution curves as function of device temperature and

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dominant conduction mechanism in the hybrid structure is also reported.

2. Experimental details

Thin film of ZnPc was deposited by high vacuum sublimation on annealed n-type silicon ⟨100⟩ single crystal wafer ($6.2 \times 10^{-3}\ \Omega$ cm resistivity) to fabricate the hybrid heterojunction. The silicon wafer was etched initially by wet chemical etching process to obtain the fresh surface of silicon wafer and to reduce its thickness to 300 microns. The silicon wafer was then cleaned in running de-ionized water, followed by a rinse in HF: H_2O (1:10) solution. Further cleaning of the wafer was carried out with IPA and acetone in an ultrasonic bath. The n-silicon surface was thus prepared and the wafer was loaded into a high vacuum evaporator of Leybold Heraeus A550 V, the heat resistive evaporation system. High purity Au–Sb (1% Sb) powder was evaporated on backside of the wafer to obtain an ohmic contact. On the front side of wafer, a layer of ZnPc, of 300 nm thickness, was evaporated, with an evaporation rate of 2A°/s. After that, 500 nm thick contact of Al on the ZnPc film was deposited through a shadow mask, to obtain the front contact area of 2.83×10^{-1} cm^2. All films were deposited at the base pressure of 2×10^{-6} mbar. The prepared structure of Al/ZnPc/n-Si/Au-Sb(1%) was characterized by *I–V–T* measurements under dark conditions in terms of its electrical properties, in the device temperature range of 283–343 K. The device temperature was maintained by using "endocal Refrigerated Circulating Bath" of Neslab Instruments Inc. and the *I–V* measurements were carried out with KEITHLEY-2420 sourcemeter with GPIB data transfer cord.

3. Results and discussions

The Al/ZnPc/n-Si metal semiconductor contact with organic layer was characterized in terms of different interrelated aspects to study its charge transport properties.

3.1. Current–voltage characteristics

The semi log plots of the *I–V–T* data of the device, in the temperature range of 283–343 K, under forward and reverse bias conditions are shown in Fig. 1. The figure shows rectifying behavior of the device. Assuming that there is a Schottky phenomenon in the device and the net current of the device is due to thermionic emission i.e. the diode is a non-ideal diode. The ideal diode equation [25] for the non-ideal diode can be expressed as [26]:

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

where n is the diode ideality factor, q is the electronic charge, V is the applied voltage, k is the Boltzmann constant, T is the absolute temperature and I_s is the saturation current given by:

$$I_s = SA^*T^2\exp\left(-\frac{q\phi_B}{kT}\right) \quad (2)$$

where S is the contact area, A^* is the Richardson's constant, equal to 110 A/K^2-cm^2 for n-type Si [25] and φ_B is the barrier height.

The n, φ_b and R_S values were determined by the standard diode characterization technique i.e. by extrapolating the linear part of semi logarithmic *I–V* plots to current axis to find the value of reverse saturation current and the value of 'n' and φ_b were determined by using Eqs. (1) and (2) respectively. The value of R_S was obtained from the slope of the semi logarithmic *I–V* plots at all device temperatures. The cross check technique of reproducing the *I–V* curves, by using the calculated values of n, φ_b and R_S in Eq. (1), was used to validate the determined values of n, φ_B and R_S parameters at all device temperatures. The good agreement between the experimental and reproduced *I–V* curves, at an intermediate device temperature of 313 K, is shown in Fig. 2 and the shift in n, φ_B and R_S values of the hybrid heterojunction, as a function of device temperature, is shown in Figs. 3–5, respectively. As a function of device temperature, the value of "R_S" is found to decrease with increasing device temperature, whereas; the value of φ_b is found to increase with increasing device temperature. This can probably be attributed to some shift in the Fermi level of the organic semiconductor, ZnPc in our case, with device temperature. The fact that the barrier height of the device increases from 0.839 to 0.939 eV i.e. by 100 meV in the device temperature range of 283–343 K, can also probably be attributed to some shift in the Fermi level of the organic semiconductor. The value of diode ideality factor increases up to the device temperature of 323 K and then decreases with further increase of temperature. This might be attributed to some shift in the proportions of the diffusion and recombination currents.

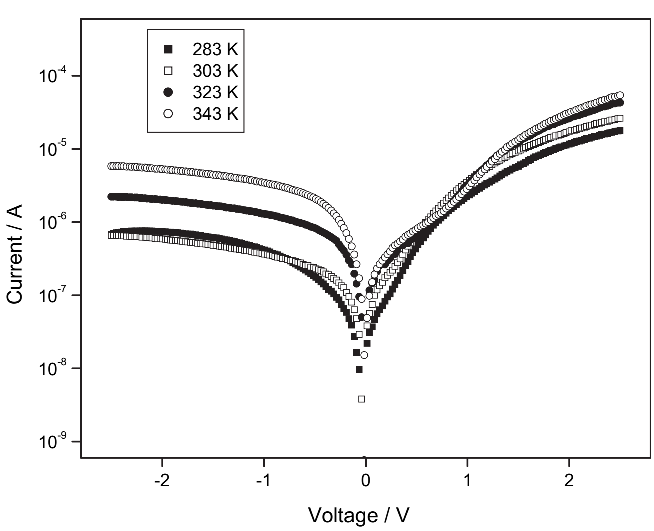

Fig. 1. Semi logarithmic plots of forward and reverse bias *I–V* characteristics at different temperatures of the Al/ZnPc/n-Si structure.

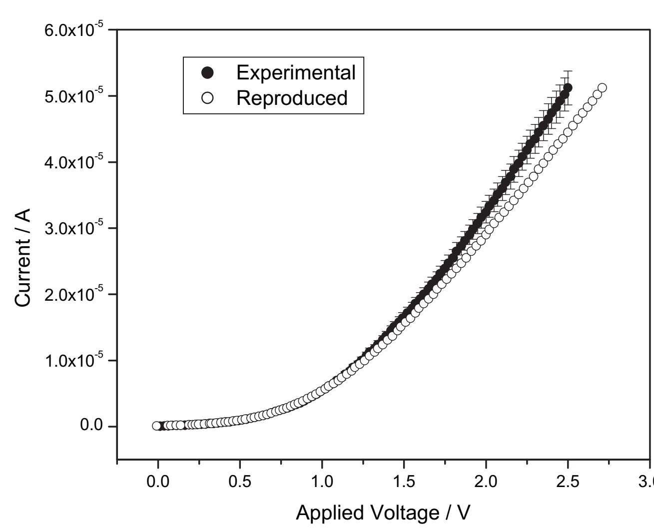

Fig. 2. Experimental and reproduced (by adopting calculated n, φ_b and R_S values in diode equation) forward bias *I–V* characteristics at 313 K of the Al/ZnPc/n-Si structure.