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Study of the Electrical Behavior of Metal/ α -SiC:H/poly-Si(N) Structure Using Simulation

P. PAPADOPOULOU^{a,*}, S.G. STAVRINIDES^b, M. HANIAS^c, L. MAGAFAS^a

^aElectrical Engineering Department, E.M.T. Institute of Technology, Kavala, Greece

^bPhysics Department, Aristotle University of Thessaloniki, Thessaloniki, Greece

^cPhysics Department, National Kapodestrian University of Athens, Athens, Greece

In this report, a study of the electrical behavior for the Metal/a-SiC/poly-Si(n) structure, appears. Different thicknesses of a-SiC:H thin films are considered; in specific the a-SiC:H layer thickness is varied between 100 Å up to 800 Å. The 2-D ATLAS advanced numerical simulator has been utilized in order to simulate the material's electrical behavior and produce the reported hereby results. The study of the I-V (current-voltage) characteristics of these Metal/ α -SiC:H/poly-Si(N) structures, reveals a very interesting hysteretic behavior that is a function of the a-SiC:H thin-film thickness. Such materials have lately raised the engineering community's interest because of their possible utilization as memristive elements.

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1. Introduction

Amorphous thin films of hydrogenated silicon carbide (a-SiC:H) have been exhaustively studied for more than 40 years, due to their interesting properties, namely extensive hardness, thermal and chemical stability, high resistance in radiations, wide optical band-gap and considerable absorption in the blue region of the spectrum. Moreover, a series of applications in the field of microelectromechanical systems [1], such as high efficiency solar cells, thin film transistors (TFTs), Schottky diodes [2] and optical sensors [3] have arisen. However, even though this structure a-SiC:H/c-Si demonstrates very attractive applications [3], only a few things have been done on the topic of isotype heterojunction [2]. In a previous paper of our team [4] the electrical behavior of such kind of junction (Al/a-SiC:H/c-Si(n)) was studied in the case of a wide band gap of amorphous semiconductor $(E_q = 2.9 \text{ eV})$ and for different values of the density of localized gap states (N) and an interesting chaotic behavior was revealed.

In this paper, a study of the electrical behavior of the structure Al/a-Si:HC/poly-Si, for different thicknesses (d) of a-SiC:H thin films (100 Å up to 800 Å), is reported. This study reveals a very interesting hysteretic behavior. Such hysteretic behaviors has attracted interest during the last years due to their possible exploitation in constructing memristors or memristive devices.

2. Simulation results

The typical structure of a Metal/ α -SiC:H/poly-Si(N) isotype heterojunction appears in Fig. 1. The a-SiC:H

thin films are amorphous, exhibiting: (i) an optical energy band gap of $E_g = 3.2$ eV, and (ii) an activation energy of dark conductivity $E_a = 0.85$ eV. It should be noted that the a-SiC:H/c-Si(n) heterojunction is assumed to be isotype, since the sputtered a-SiC:H has been found to present an n-type behavior [5]. Its electrical behavior was investigated by utilizing the 2-D ATLAS advanced numerical simulator by simulating the I - V (current-voltage) characteristics.



Fig. 1. Typical structure of a Metal/a-SiC/poly-Si(n) isotype heterojunction.

In Fig. 2, the current (I) versus bias voltage (V_{bias}) of the a-SiC:H/poly-Si(n) isotype heterojunction for different thicknesses of the amorphous semiconductor, is presented. Under forward bias conditions the polarity is negative to the a-SiC:H side of the junction. It is clear from this figure that the I - V curves as the applied bias voltage (V_{bias}) was gradually changed from the value of $V_{bias} = 0.0$ V to the value of $V_{bias} = 0.8$ V and then backwards, the current values through the device did not get the same values for the same applied bias voltage, in both directions; thus demonstrating an interesting hysteresis effect. This hysteretic phenomenon got more intense as the thickness of the a-SiC:H thinfilms was decreased from 800 Å (Fig. 2e) down to 100 Å (Fig. 2a), through three steps namely 600 Å, (Fig. 2d) 300 Å, (Fig. 2c) 200 Å, (Fig. 2b). For higher thickness

^{*}corresponding author; e-mail: ppapado@teikav.edu.gr



Fig. 2. I-V characteristics of the a-SiC:H/poly-Si(n) isotype heterojunction for five different thicknesses of the a-SiC:H thin-film: (a) 100 Å, (b) 200 Å, (c) 300 Å, (d) 600 Å, (e) 800 Å. Note that for higher thin-film thicknesses the hysteretic phenomenon is being suppressed and almost vanished.

values the hysteresis phenomenon disappears. The described behaviour provides this device with an attribute analogous to that of classic memristors, i.e. the hysteresis phenomenon intensity changes according to the device's thickness whereas in classic memristors it changes according to the frequency of the applied voltage or current signal.

3. The proposed model

The typical structure of a Metal/a-SiC/poly-Si(n) isotype heterojunction and its energy band-diagram both under thermal equilibrium, as well as under forward- bias conditions appear in Fig. 3. This energy band-diagram was calculated using Anderson's model [6]. The conductivity of the a-SiC:H was considered to be of n-type, as it was found in our earlier study [4], and it has been confirmed by the present work.

In this figure, subscript 1 refers to a-SiC:H, while subscript 2 to poly-Si(n). In this way, E_{C1} and E_{C2} are the edges of the corresponding conduction bands; E_{V1} and E_{V2} are the edges of valence bands; E_F is the distances between the Fermi level and the corresponding conduction band edges and E_{g1} , E_{g2} the energy band gaps.



Fig. 3. Metal/a-SiC/poly-Si(n) isotype heterojunction.

Taking into account that the Metal/a-SiC:H is an ohmic conduct, the whole structure realizes an isotype potential barrier to the a-SiC:H/poly-Si(n) junction. As the forward bias voltage increases, the edge of conduction band E_{C1} moves towards higher values, whereas E_{C2} remains almost constant. This is anticipated, since the a-SiC:H/poly-Si(n) isotype heterojunction is an one-sided junction (the value of the effective density of localized gap states in a-SiC:H $N_1 = 5 \times 10^{15} \text{ cm}^{-3}$ is significantly lower than the donor impurities $N_2 = 5 \times 10^{18} \text{ cm}^{-3}$ in poly-Si). More specifically due to the fact that the a-SiC:H thinfilm demonstrates an energy band-gap $E_{q1} = 3.2 \text{ eV}$, thus behaving as a semi-insulator. As a result, a small number of electrons from the extended states of the conduction band of the a-SiC:H side, have the ability to surpass the junction potential barrier more easily than electrons from the poly-Si(n), contributing to the main current component, which is a low level current.

At the same time, as the forward bias voltage increases, electrons induced on the Al/a-SiC:H side and can be transported, via the localized gap states near the Fermi level, from the a-SiC:H side to the poly-Si(n) side, through a tunneling mechanism to the conduction band of poly-Si, thus also contributing to the forward current. However, this current contribution presents a time delay and this is the reason why a hysteresis phenomenon emerges, which is clearly observed in the forward I - V characteristics, appearing in all five figures in Fig. 2. This was verified by the fact that as the rate of forward bias decreases the hysteresis phenomenon deteriorated.

4. Conclusion

The present study of the electrical behavior of the a-SiC:H/poly-Si(n) isotype heterojunction, through the forward I - V characteristics, revealed a very interesting hysteretic phenomenon, which depends on the thickness (d) of the a-SiC:H thin film, while it disappears as d becomes greater than 800 Å. This hysteresis phenomenon can be explained by the fact that the amorphous semiconductor, in the whole structure (Metal/ α -SiC:H/poly-Si(N)), operates as an insulator in a capacitor. Initially, as the bias voltage increases a low forward current is observed, due to the low level conductivity of a-SiC:H thin film. When electrons induced on the Al/a-SiC:H side, they can be transported, via the localized gap states near

the Fermi level, from the a-SiC:H side to the poly-Si(n) side, there is another current component contributing to the total forward current. Finally, as d increases, the hysteresis phenomenon weakens and this is due to the fact that it is more difficult to transport electrons from metal to poly-Si(n) via the a-SiC:H thin film. Due to this hysteretic phenomenon the a-SiC:H/poly-Si(n) isotype heterojunction could be considered to be a very interesting device in constructing memristors or memristive devices.

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