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a-Si_xGe_{1-x}:H thermoelectric thin film Schottky diodes: characterization and applications

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ABSTRACT: *The characterization of the thermoelectric properties of nanostructured a-Si_xGe_{1-x}:H thermoelectric thin film deposited by PECVD through the use of Schottky diodes formed by placing a metal in contact to the material is presented. The use of a green laser for locally heating the material is presented and compared with the measurements performed in a Variable Temperature MicroProbe System, the results show that even the thermal conductivity measured by the 3□ method are very similar to the results here obtained. For obtaining the thermal and thermoelectric properties of a thin film the TERM-PRU-MA1 microchip was designed, containing structures that allow us to characterize a thermoelectric material thin film.*

KEYWORDS *Thermoelectric power, Schottky diode, characterization, nanostructured thin film, Energy harvesting.*

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I. INTRODUCTION

Thermoelectric materials had been a studied topic recently, this is because we had achieved the limits of conventional energy sources, and it's necessary to find new ways of harvest the available energy. Energy harvesting is the process by which energy is derived from external sources is captured and stored for small, wireless autonomous devices. Thermoelectric phenomena have been a topic of technological interest due their possibilities of transforming the wasted thermal energy from devices in useful energy. Thermoelectric generators (TEG's) can be used in machines or devices with medium or high heat generation. A temperature difference ΔT in the ends of a thermoelectric material will lead to the generation of a small voltage at the ends of the material [1], this is the Seebeck effect, the heart of thermoelectricity. Energy harvesting technology is fundamental for the development of "zero power" (no batteries) sensor networks, the implementation of Internet of Things (IoT) technologies and machine to machine (M2M) communication. The use of this technology in low power consumption and high efficiency sensors or electronic circuits has a potential use in different areas e.g. health care, agriculture, vital signs monitoring, security, localization or stock control [2].

Some of the advantages of thermoelectric conversion of energy are the development of compact eco-friendly solid-state devices, without mobile parts and the use of localized heat in sensors, devices or machines [3]. Studies have shown that in electronic devices 60% of the energy is lost, most in the form of residual heat. However, the efficiency of thermoelectric conversion is low and is limited mainly by the performance of thermoelectric materials.

Since the middle of the XX century, after Ioffe first proposed the research and application of semiconductor materials, alloys based on the Bi_2Te_3 or $Si_{1-x}Ge_x$ they soon became some of the most widely studied and optimized thermoelectric materials to date [4]–[6]. Standard modules for thermoelectric generators (TEG) normally use bismuth telluride (Bi_2Te_3) for its high efficiency at room temperature and its ease of deposit in the form of thin films, to make the module flexible [7]. However, the low abundance of Bismuth is a problem for manufacturers [8]. In addition, Tellurium is the ninth most rare element on earth whose prediction of depletion is planned for 2020 with current use, so it is important to find Te-free materials that are cheap and high efficiency [9].

The efficiency of thermoelectric devices is closely associated with the dimensionless figure of merit ZT ($=S^2\sigma T/\kappa$) [10]. A high-performance material has a ZT value close to or greater than 1. To achieve this, it is necessary that it has a high Seebeck coefficient (S or α), a high electrical conductivity (σ) and a low thermal conductivity (κ).

Crystal semiconductors, such as SiGe, compatible with CMOS technology have been proposed as an alternative. Some of the optimization attempts include approaches such as doping [10], [11] and nano structuring in the form of heterostructures and nanowires [12], [13] trying to increase their efficiency by introducing grain limits and point defects, which effectively increase the dispersion rate of the phonons and reduce the thermal conductivity of the network [14]. However, the results presented for ZT values are only 0.034 [10], 0.01-0.02 [12] and 0.135 [13], respectively, at room temperature. Another proposed approach is to obtain complex crystalline structures to separate the electron crystal from the phonic glass. J. Tang et al [15] propose the structure called "porous silicon" with which it is possible to obtain a network thermal conductivity (1.14-2.03 W/m·K), approaching that of amorphous silicon, with a ZT value of ~ 0.4 to 300K.

As thermoelectric modules (TEMs) are formed by the union of a metal and a semiconductor, the implementation of the Schottky voltage on the thermoelectric equations is proposed. It has been shown that the change in the height of the barrier between amorphous silicon and metal contacts in solar cells, influence the performance of them therefore, in this work it is proposed to study the role of the height of the barrier between metallic contacts and thermoelectric material. Recently [25], a novel N-type amorphous silicon-germanium thin films with embedded nanocrystals has been proposed as a cheap and abundant thermoelectric material and, it is used for studying the influence of the barrier height on the thermoelectric generator performance

II. THERMOELECTRIC THIN FILM

In this work, the PECVD synthesis of the high-performance nanostructured thermoelectric material based on a highly doped N type a-SiGe:H is presented. As the properties of the material are a function of the deposit conditions such as pressure, gas flow ratio, temperature, power, among others, these are optimized for obtaining the a-SiGe alloy with the highest conductivity. Then, the samples were submitted to a heat thermal annealing of 500°C for 30 minutes and an increase of 3 orders of magnitude in conductivity with reference to the un-annealed samples is obtained, but the amorphous network is conserved. The details of the deposition parameters, electrical, thermal conductivities and Seebeck coefficient are published elsewhere [25].

III. CHARACTERIZATION

In order to know in the deposited films some important properties such as activation energy (E_A), the thermal coefficient of resistance (TCR), and electrical resistivity the relationship of the current-voltage ratio (I (V)) as a function of the temperature is used. For this purpose the a-SiGe:H was deposited onto corning glass (2974) substrates, the Ti electrodes were deposited by e-beam to realize electrical characterization. The surface roughness and thickness were measured by profilometry. On the other hand, the deposits made on corning glass (1737) and high resistivity silicon are used for optical characterization, as well as composition analysis using the technique of infrared Fourier transform spectroscopy (FTIR). Here we present some of the characterization techniques used. The SiGe:H thin films were analyzed on an FTIR spectrophotometer (model Vector 22, Bruker) to know the molecular composition of the films deposited in the range of 400 to 2500 cm^{-1}, to determine the Si-H and Ge-H bonds present. To determine surface roughnessof the material, an AFM Nanosurf Easy Scan 2.3 microscope was used to scan 2x2 areas up to 50x50μm^2.

IV. THERM-PRU-MA1 MICROCHIP

For determining the electrical and thermoelectric properties of a thin film and its related figures of merit, and for the fabrication of Schottky diodes with metal and the a-SiGe:H, test structures are necessary that guarantee the measurement of the Seebeck coefficient and the figure of merit ZT quickly and reliably. That's why the TERM-PRU-MA1 microchip was designed, which includes different electrical, thermoelectric and mechanical test structures.

The microchip contains microheaters and micro thermometers, the latter can be platinum or Schottky diodes, depending on the chosen manufacturing process. Likewise, thermally insulated structures are included by a micromachining process using KOH. Some of the structures included in the TERM-PRU-MA1 microchip are described:

A. C1 & E1 structures

With these structures (Fig 1.a), reported in [17], the Seebeck coefficient and the Peltier effect can be measured.

B. A1 & B1 structures

The purpose of this structure is to measure the Seebeck coefficient, heating one end of the strip of material to cause a ΔT between both ends, and measure the generated ΔV. They are seen in fig. 1.b

C. D2 & E2 structures

These structures designed for the calculation of thermal conductivity and proposed in [18], must be thermally insulated by micromachining, suspended on a thin Si_3N_4 membrane. The structures are seen in Fig. 1.c.

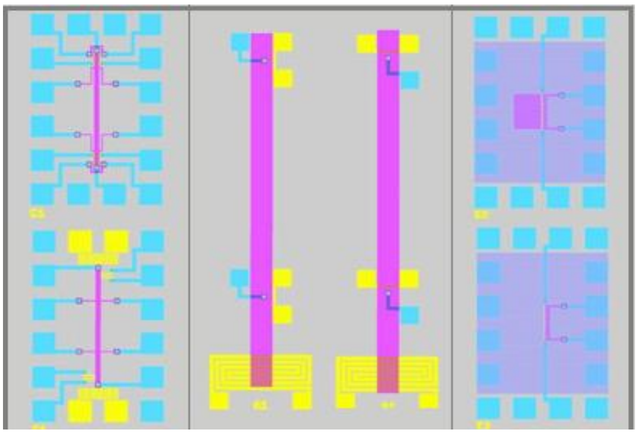


Fig. 1. Tests structures (a) C1 & E1, (b) A1 & B1 and (c) D2 & E2.

V. THE SCHOTTKY DIODE

The Schottky diode or barrier diode is named in honor of the German physicist Walter H. Schottky. In most diodes, the metal is generally deposited in an N-type material.Schottky diodes use the metal-semiconductor junction due to the behavior of the work function. As it is known, the work function is the minimum energy required to move an electron from the Fermi energy level to the vacuum. In this work Shcottky diodes were fabricated by placing metallic contacts to the a-SiGe:H films

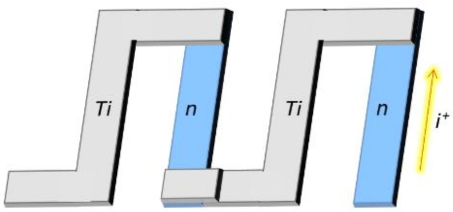
As mentioned earlier, it has been shown in solar cells that the change in the height of the barrier between amorphous silicon and metal contacts, has an influence on its performance [19], and that is why, similarly, it’s intended to study the role of the barrier height between the metallic contacts and the proposed thermoelectric material in order to prove if it is possible to improve the thermoelectric generation by means of the correct selection of the contact metal, reflected in the open circuit voltage.

There are many factors that determine the height of the Schottky barrier, among these factors are the difference in work functions between the metal and the semiconductor, the distribution of surface states, and the nature of the interface and the electric field on the surface of the semiconductor. In this work it is proposed to select the metal with the ideal work function to increase the barrier height.

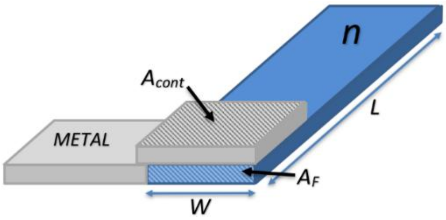
VI. TEG EQUATIONS

Considering the proposed design for the planar thermoelectric generator (TEG) in Fig. 2.a, it is observed that there is a metallic contact at each end of the strip, which generates a Schottky-type junction with the proposed n-type thermoelectric material. This junction also generates contact resistance, which must be also considered.

A schematic diagram showing values of interest is shown in Fig. 2.b. The dimensions of the strip are W in width, L in length and Th in thickness. The cross-sectional area of the A_F strip consists of the product of the width W and the film thickness Th. The area A_{cont} is the area of the contact between the metal and the thermoelectric material.



l)



(b)

Fig. 2. (a) Proposed thin film planar TEG and (b) detail of the metal-thin film junction of the TEG.

By Ohm's law, the output power of a TEG connected to a resistive load is I^2R_L, where R_L is the resistive load. Considering the contact resistance R_C at the interconnections and the Schottky voltage V_{Sch}, at a given ΔT the current through a TEG with N strips of resistance R and the output powerare:

$$I = \frac{N(\alpha\Delta T + V_{Sch})}{R_L + N(R + R_C)} \tag{1}$$

$$W_s = \left[\frac{N(\alpha\Delta T + V_{Sch})}{R_L + N(R + R_C)}\right]^2 R_L \tag{2}$$

respectively. The maximum current I_{MAX} and maximum power W_{smax} are:

$$I_{MAX} = \frac{\alpha\Delta T + V_{Sch}}{2(R + R_C)} \tag{3}$$

$$W_{smax} = \frac{N(\alpha\Delta T + V_{Sch})^2}{4(R + R_C)} \tag{4}$$

when$R_L = N(R+R_C)$. The TEM's efficiency in the presence of contact resistance is:

$$\eta = \frac{R_L N A^2}{B A\alpha T_H - B^2 K(T_C - T_H) - \frac{(R+R_C)N^2A^2}{2}} \tag{5}$$

Where $A=(\alpha\Delta T+V_{Sch})$ and $B=(NR+R_L)$ and T_C and T_H are the temperatures of the cold and hot side of the strip. The efficiency corresponding to W_{MAX} is:

$$\eta_{wm} = \frac{N^2A^2Z_C(R + R_C)}{Z_C A\left(\alpha N T_H - \frac{A^2}{4}\right) - 2\alpha^2(T_C - T_H)} \tag{6}$$

where$Z_C = \alpha^2/K(R+R_C)$. If T_M is the average of T_H and T_C, maximum efficiency occurs when $R_L = \gamma_C NR$, where $\gamma_C = \sqrt{(1 + Z_C T_M)}$, and is given by:

$$\eta_{MAX} = \frac{\gamma_C A^2}{AC\alpha T_H - C^2K(R + R_c)(T_C - T_H) - \frac{A^2}{2}} \tag{7}$$

In terms of η_C:

$$\eta_{MAX} = \frac{\gamma_C A^2}{AC\alpha\Delta T - C^2K\Delta T(R + R_c)\left(\frac{T_C}{T_H} - 1\right) - \frac{\Delta T A^2}{2T_H}} * \eta_C \tag{8}$$

where$C = (\gamma +1)$. The corresponding current and power output are:

$$I(\eta_{MAX}) = \frac{(\alpha\Delta T + V_{Sch})}{(R + R_C)(1 + \gamma_C)} \tag{9}$$

$$W_s(\eta_{MAX}) = \frac{N\gamma}{R + R_C}\left[\frac{\alpha\Delta T + V_{Sch}}{1 + \gamma_C}\right]^2 \tag{10}$$

VII. SCHOTTKY DIODE EXPEWRIMENTAL PROCESS

The selection of the metal is of the utmost importance for the increase of the open circuit voltage of the junction, since depending on the work function of the metal, it will be the height of the Schottky barrier and therefore the magnitude of said voltage.

For a priori metal selection, based on the work function and availability and behavior it was decided to perform tests with titanium (φ≈4.33ev) and platinum (φ≈5.65ev).For the fabrication of the structures to be characterized, it is proposed to use the diode design included in the TERM-PRU-MA1 microchip, which has structures useful for the characterization of Schottky diodes. The microchip also has structures to measure the electrical, thermal and thermoelectric properties of the materials from which the diode is manufactured, including contact resistance.

Some of the structures require thermal insulation, which is why a micromachining process was designed to leave them suspended in a Si_3N_4 thin film.

There are numerous characterization methods to obtain the height of the barrier in a Schottky junction. The methods used in this work are described below.

a. I-V –T characteristics.

These I-V measurements are carried out in a Variable TemperatureMicroProbe System.

The purpose of these measurements is to observe the influence of the thermoelectric material on a Schottky diode at different temperatures. This is also a quick test to see the effect of the selected metal and the quality of the diode.

In Fig. 3 the characteristics I-V for a diode formed by the union of a-SiGe with Titanium for a temperature range, from 300K to 370K, are shown.

The increase in the value of the current is observed when the temperature increases, despite still having very small values due to the selected materials and the size of the structures.

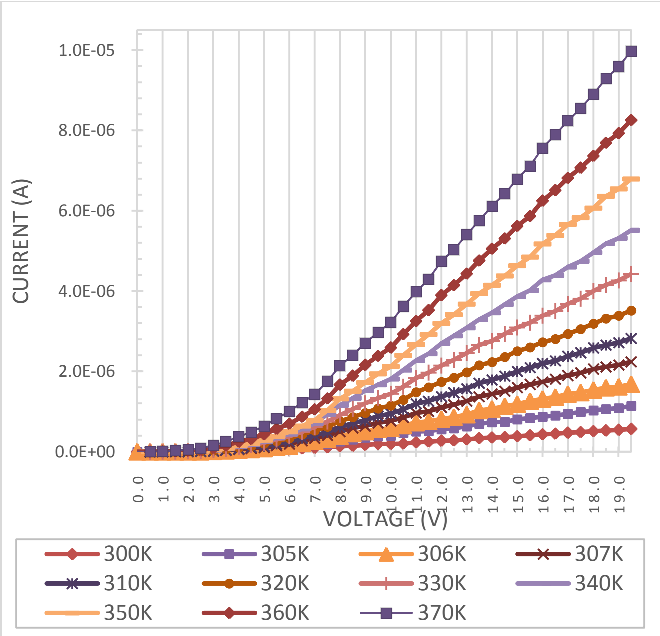


Fig. 3. a-SiGe/TitaniumSchottky diode I-V characteristics for different temperatures.

As explained in [20], the J-V_a characteristics of a Schottky junction can be adjusted using the diode equation:

$$J = J_s[\exp(qV_a/nkT) - 1] \quad (11)$$

Where J is the current density (J = current/effective area), V_a is the voltage applied along the junction, q is the charge of the electron, k is the Boltzmann constant, T is the absolute temperature, n is an empirical constant and Js is the saturation current density. Therefore, from the J vs V_a graph, both n and Js can be obtained. Then the height of the barrier φ_B can be obtained with the Richardson equation:

$$J_s = A^* T^2 \exp(-\frac{q\varphi_B}{kT}) \quad (12)$$

It is noted that Richardson's constant can be obtained by measurements at different temperatures or by consulting tables.

From equation 11, the voltage drop V_D can be expressed as the serial connection of a diode and a resistor, so V_D = V-IR, so for V_D> 3kT/q:

$$I = I_s \exp[q(V - IR)/nkT] \tag{13}$$

Taking $J=I/A_{eff}$:

$$V = RA_{eff}J + n\varphi_B + \left(\frac{n}{\beta}\right)\ln\left(\frac{J}{A^*T^2}\right) \tag{14}$$

Where:

$$\beta = q/kT \tag{15}$$

Deriving equation 14 with respect to J, and rearranging terms, we obtain:

$$\frac{d(V)}{d(\ln J)} = RA_{eff}J + \frac{n}{\beta} \tag{16}$$

So, the d(V)/d(lnJ) vs J graph will give us RA_{eff}as the slope and n/β as intercept on the y axis. To evaluate φ_B, a function H(J) is defined:

$$H(J) \equiv V - \left(\frac{n}{\beta}\right)\ln(J/A^*T^2) \tag{17}$$

From equation 14 we can deduce:

$$H(J) = RA_{eff}J + n\varphi_B \tag{18}$$

Using n obtained from equation 16, the graph H(J) vsJ will give us a line with an intercept of value $n\varphi_B$ on the y-axis. The slope of this graph gives us a second determination of R, used to verify consistency. Therefore, by making two different graphs of the J-V data of a single measurement, the three key parameters of the diode can be obtained: n, R and φ_B. Details of this method can be seen in [21].

VIII. RESULTS

Through High Resolution Transmission Electron Microscope (HRTEM), it was observed that the a-SiGe thin film has nanometric structures with a grain size between 15 and 25 nm as depicted in figure 5, the nanostructures that the material possesses as well as the thin film effects improve the thermoelectric properties of the material [23].

Schottky diodes were used as micro thermometers during the thermoelectric material characterization process. Thanks to the implementation of a green laser as a heat source, real-time hot spot temperature and Seebeck voltage can be obtained in a single measurement process. A green laser was selected for its wavelength size, ≈ 550 nm, comparable to the thickness of the thin film of interest. A constant temperature on the laser spot was achieved pulsing the laser via optical chopper.

Calibration tests using the micro thermometers were carried out to find the optimum powers, times, and modulation values to carry out the experimental processes mentioned above, some of these calibration processes can be seen in Fig. 4, where the sample was heated at a controlled and specific temperature, and several I-V characteristics were measured in the micro thermometer. Then, using the focused laser on the micro thermometer, I-V characteristics were measured again to compare results and therefore calibrate the laser heat source. The temperatures selected for the study correspond to temperatures of interest for power devices used in room temperature applications.

The results of the thermoelectric measurements and ZT calculation of the a-SiGe thin film are shown in Table II, where ρ is the electrical resistivity, σ is the electrical conductivity, κ is the thermal conductivity and S_{avg} is the average Seebeck coefficient for each temperature. The behavior of ZT corresponds to the expected behavior of a material with the same characteristics [24].

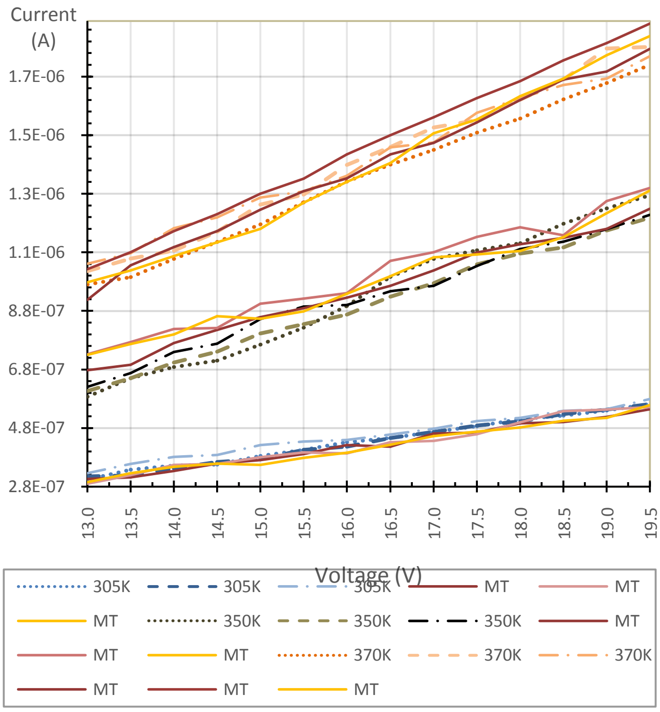


Fig. 4. Micro Thermometers I-V characteristics for temperature measure references (Ref) and during thermoelectric measurements (MT m.).

TABLE II
ZT CALCULATED FOR SAMPLE 4

ΔT	5.5	50	70	K
ΔV avg.	0.03233	0.2826	0.4162	V
ρ	8	8	8	Ω * cm
σ	12.5	12.5	12.5	S / m
κ	0.58	0.52	0.5	W/mK
$\kappa_{3\omega}$	0.57	0.53	0.51	W/mK
S avg.	0.00587	0.005652	0.005946	V / K
T	302.5	325	335	K
ZT	0.2252	0.2496	0.2961	-

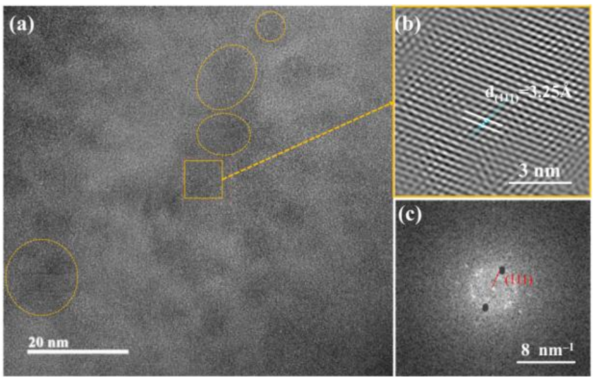


Fig. 5. (a) The cross-section of the representative sample in high-resolution mode (HRTEM), (b) single nanocrystal of SiGe alloy, and (c) fast Fourier transform patterns of the nanocrystal.

IX. CONCLUSIONS

Through HRTEM, it was observed that the material has nanometric structures with a grain size between 15 and 25 nm, as seen in figure 5. The conditions that lead us to high deposition ratios also lead us to a nanostructured material. The nanostructures that the material possesses as well as the thin film effects improve the thermoelectric properties of the material [25].

The resulting material has been electrically characterized. Schottky diodes were included in the TERM-PRU-MA1 microchip to obtain their I-V characteristics at different temperatures and use them as micro thermometers. These micro thermometers were calibrated using precise temperature control.

Analytical analysis of the thermoelectric equations considering the Schottky voltage were made to optimize the generator design.

Heating the test structures with a focused laser was proposed and tested. Calibration to find the laser and chopper properties were made using the micro thermometers. Results of the thermoelectric characterization obtained are shown in table II show an expected behavior and the κ values are close to the 3ω technique used by Ascencio et al. [10] for the same material.

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