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Theoretical Study and Modeling of Porous Silicon Gas Sensors

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Abstract
In this work ,porous silicon(PS) substrate has been used to fabricate a sensor of structures(Al/n PSi/n-Si/Al) using infrared laser in a assisting Etching process at several times (8,16,and24 min) and current density(J) of about(25mA/cm2) on silicon(Si) substrates type of n and tested for CO2 gas molecules and then modulated using MATLAB program. J-V characteristic was analyzed. Different parameter determine such as, Porosity (%), Layer thickness (%) and relative permittivity of the fabricated PS substrate. Several shape and sizes of pores were obtained from the scanning electron microscope device such as pore, rectangular and cylindrical structure for infrared illuminated (IR). The Porosity (%) and Layer thickness (%) take control on sensing mechanism.

Keywords: porous silicon, gas sensor, carbon dioxide

دراسة نظرية و محاكاة للمتحسسات الغازية للسيليكون المسامي

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الخلاصة
في هذا العمل، تم تصنيع متحسس غازي من السيليكون المسامي على (Al / n PSi/ n-Si / Al) باستخدام ليزر الأشعة تحت الحمراء واستخدم عملية الحفر الليزري عند كثافة تيار ثابتة حوالي 25 ملي امبير/سم^2 واوقات حفر مختلفة (8،16 ، و 24 دقيقة) على مادة السليكون نوع n ومن ثم اختبارها باستخدام جزيئات غاز ثنائي اوكسيد الكاربون ومحاكاته باستخدام برنامج الماتلاب. وتم حساب خصائص كثافة التيار– الفولتية ,المسامية,سمك الطبقة , وثابت العزل الكهربائي الفعال لطبقة السليكون المسامي.اوضحت صورة مايكروسكوب الماسح الضوئي تكون المسام بشكل حفر دائرية واسطوانية ومستطيلة الشكل ذات ابعاد مختلفة بالأشعة تحت الحمراء. إن آلية الاستشعار تحكمها سمك ومسامية طبقة السليكون المسامية.

Introduction

Porous silicon is a very promising material in many applications for many reasons like its unique combination of crystalline structure, its large surface area to volume ratio, high activity in surface chemical reaction, capability to produce several morphologies, and low power usage of porous silicon based sensor compared to other sensors. Silicon (Si) crystalline skeleton have a net of nanosized voids

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leading to the formation of a sponge structure of distribution channels [1]. Laser assisting Etching process is one of the most important techniques for PS formation Focusing
The laser on the upper surface of silicon results
in the absorption light and more reduction in size to obtain the micro and macro PS structure which depends
on the laser wavelength [2,3]. The overall interaction is shown by the following equation [4]:

$$Si + 6HF \longrightarrow H_2SiF_6 + H_2 + 2H^{+} + 2e^{-} \quad \text{.....................(1)}$$

Carbon dioxide co_2 sensing is common at present because of its high presence in air. Optical properties usually control the sensing mechanism of gas but it is very expensive [5, 6]. There are many reasons for using porous silicon (PS) instead of silicon (Si) crystals such as its high resposivity in the sensing application, easy and unexpensive manufacture. Etching mechanism and several morphology can be obtain, and different techniques can use to read the result [7]. Activation of trapping center due to adsorbate interaction with dangling bond state can explain conductance variation due to the trapping or release of carrier. Furthermore, the molecules of CO2 act as accepter centers.

Fabrication of test device

A commercially available Si substrate (100) n-type of resistivity (10Ω.cm) and thickness (625µm) has been used. After cutting the silicon substrate into (1*1 cm) the pieces were immersed in Ethanol diluted with Hydro Fluoric acid (HF) in the rate of (1:10) to clean it from the oxide layer. The specimen was washed with water and left outside for a few minutes to dry. Finally they were stored in a container and immersed in Methanol to avoid oxide formation. The etching solution was a mixture of (HF:Ethanol) in a ratio of (1:1),the concentration of hydrofluoric acid was equal to(24%). Ethanol is usually used to avoid aggregation of hydrogen bubbles. Power supply, Ammeter, Teflon cell, and laser source were also required for the experimental workInfrared laser is of (810nm)wavelength,and(2W/cm2)intensity has been used. Aluminum (AL) electrode of thickness (5-20nm) was deposited on the upper and lower surface of porous silicon specimen after the preparation mechanism. As shown in Figure-1.

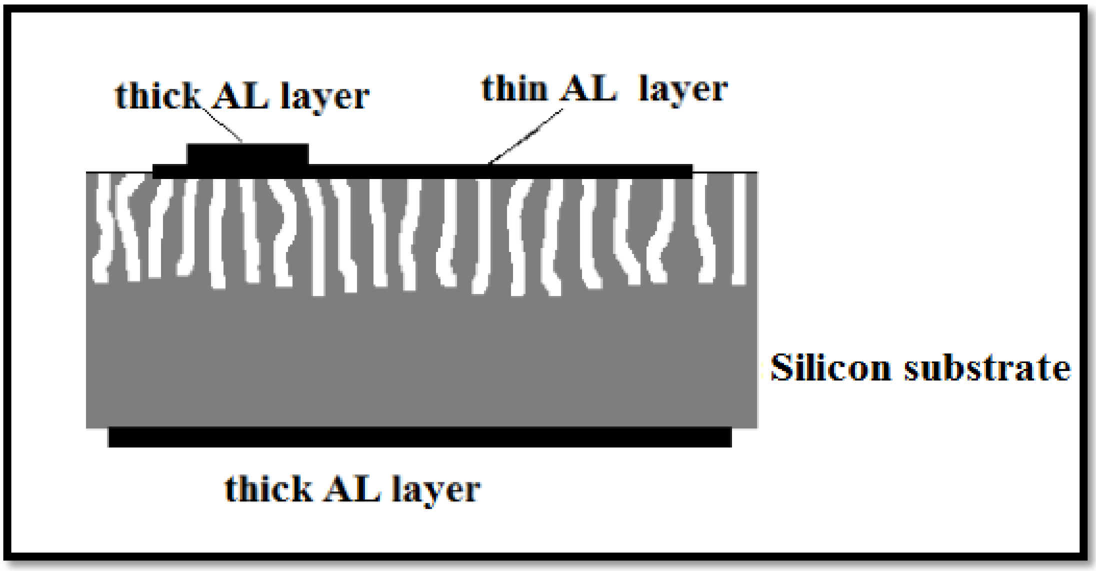


Figure 1-PS gas sensor device.

Results and Discussion

1. Porosity (%) and Layer Thickness

Porosity(%) is one of the most important features in the porous silicon.This parameter illustrates the amount of void in the silicon substrate which change to new material with different properties from the substrate[8].The porosity(%) and layer thickness(%) is determine form the following equations where, P1 is the porous silicon specimen mass before etching , P_2 is the porous silicon specimen mass after etching and P_3 is the specimen mass after removing the porous silicon layer using Na OH solution, ρ is the silicon(Si) substrate density[9]:

$P = (P_1 - P_2) / (P_1 - P_3)$ ………… (2)

$d = (P_1 - P_3) / (\rho \times A_{PSi})$ ………… (3)

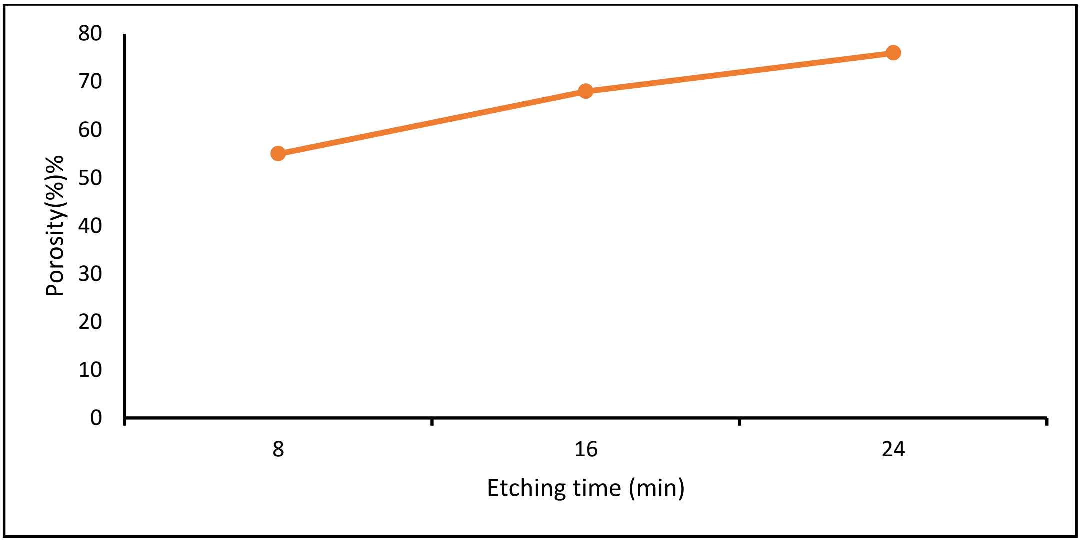


Figure 2-Show the relationship between the Porosity and Etching time.

As shown in Figure-2 a linear increase can be observed between Porosity (%) and etching time after reaching to specific value of about 76%. Fragile and weak properties results after increasing the etching time to higher than 24min. Deeper penetration into silicon(Si)substrate occur with increasing the etching time which produce more pore channel[10].

The following figure show the relationship between the layer thickness(%) and the etching time.A high value of the layer thickness(%) of about (36µm) results in the increase of the absorption depth(D) tos about(12.9µm) for IR laser. penetration depth(D) increase with increasing the wavelength of the laser . More electron-hole pairs are generated by the etching mechanism.

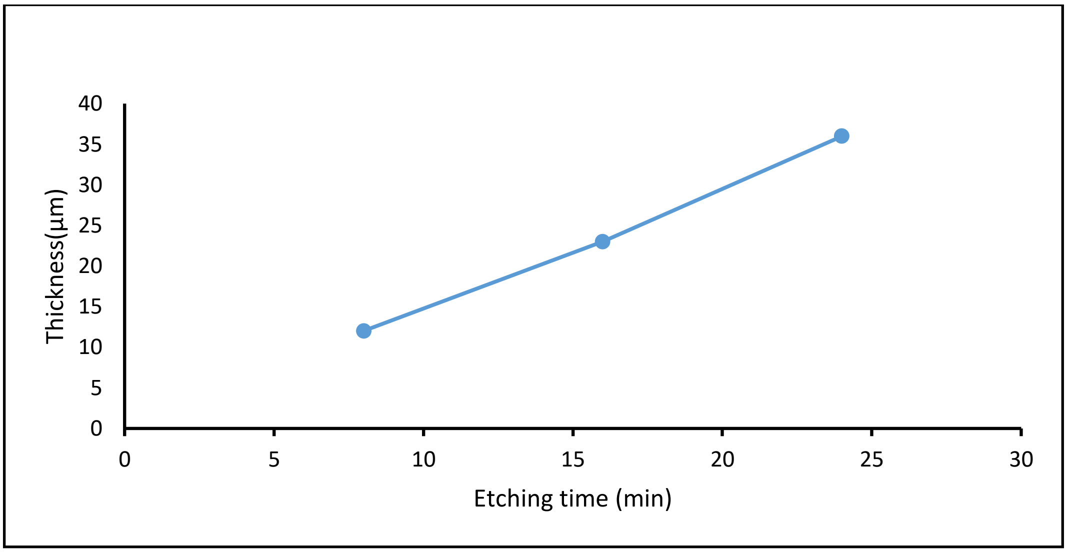
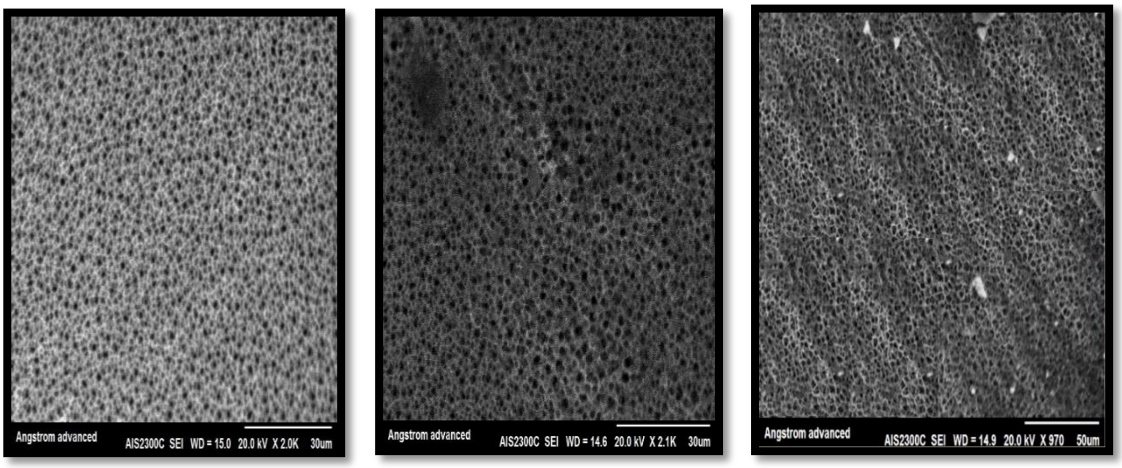


Figure 3-The relationship between the layer thickness and etching time.

2. Morphological Properties

Pores in silicon formed during the etching process depend on several parameters such as illumination wavelength (λ), etching time, laser intensity, current density, substrate type and resistivity. Pore like structure is the common shape usually obtained in the etching process. The nano-size decreases with the depth of layer of porous silicon. The Gaussian profile of the laser beam used in the etching process has an influence on the etched surface. The removing rates reduced from the center of the laser beam to the termination. The surface morphology of the specimen at several etching times 8,16 and 24 min are shown in Figures-(4.a), (4.b), (4.c).



(a) (b) (c)

Figure 4-(a, b, c): Scanning electron microscope images (top-view)of IR illustrates PS prepared at 8,16,24 min respectively.

These figures show that nano-and micro structure PSi were obtained using photo-electro chemical etching , which caused the fprmation of a regular structure and also a macroporous layer . HF solution makes deeper pores in the silicon substrate with nano sized pores ranging between (50nm_100nm) for various formation conditions.

3. Optical Properties

The optical properties of PS are different from those of the silicon substrate. The nano sized pores give strong luminescence at room temperature. The wavelength (λ) of the emitted light depends on the porosity of PS. Photoluminescence (PL) is a result of the recombination of electron-hole quantum confined. Emission from PS is an interesting property varied according to the fabrication conditions. PS emitted radiation wavelength is in the range of (UV-IR)[11]. Photoluminescence (PL) is defined as the inverse to the absorption process. Emitted light from the PS has limited wavelength (λ), in contrast with semiconductors material which emitt radiation of several wavelengths (λ). Efficient emission of visible light has been observed from silicon nanostructure [12]. The Photoluminescence (PL) properties of PS are show in the Figure-5.

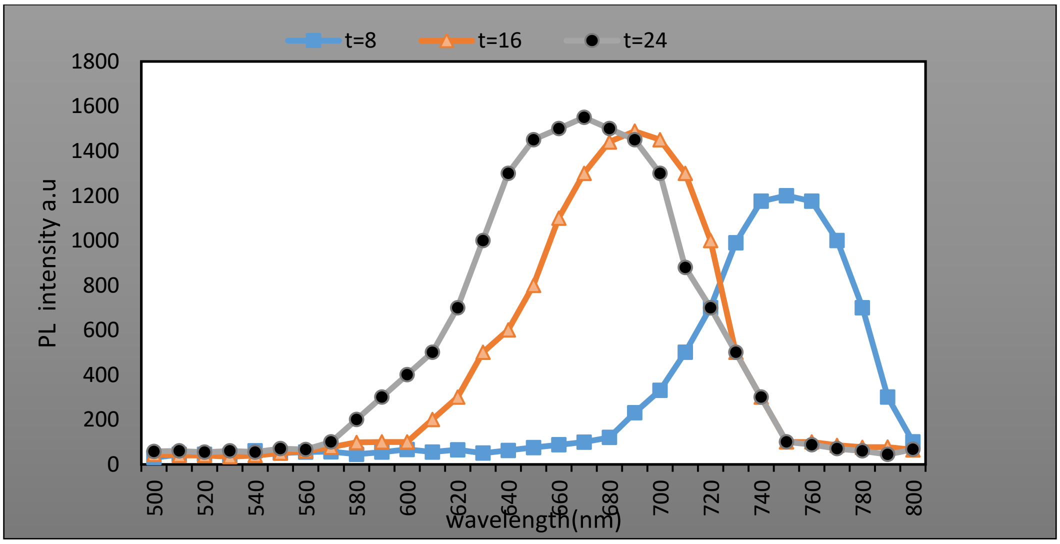


Figure 5-The Photoluminescence (PL) spectra of PS at different etching times of 8, 16,24min.

4. Gas Sensor Measurement

Many researches show that the optical electrical and chemical properties change because of the gas adsorption at the porous silicon surface or maybe due to pore full.This means that the gas adsorption or condensation in pore can be used to improve the gas sensor system. It was founded that the J-V characteristic is sensitive to different gases based on the chance of free carrier concentration in the silicon channel directly under the porous sensing layer that results from the interaction of gas molecules with PS pores. Two mechanisms are responsible for this interaction (1)change in the distance of charge region by charge redistribution and(2) change in the width of conductive channel . The following figure show the J-V characteristic for different etching times (8, 16, 24 min) at (5volt) using homemade device at room temperature.

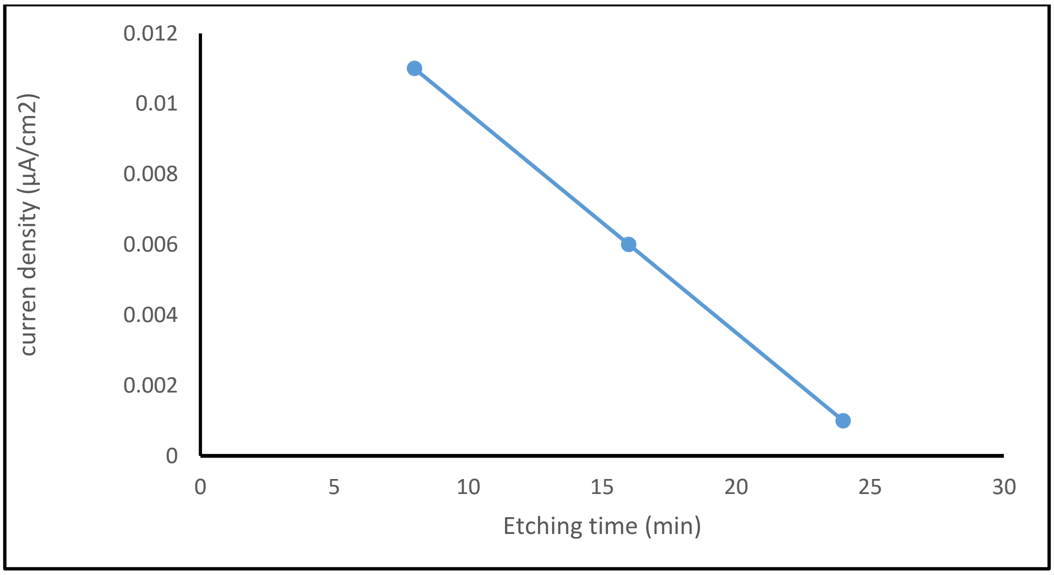


Figure 6-The relation between the current density and etching time

Experimental

The adsorbed gas molecules change the current density according the following equation

$$\mathbf{I_{PSi}= \epsilon_{rPSi}\, \epsilon O\, \mu_{eff}\, V^2/d^3} \quad \text{……………(4)}$$

Where ϵ_{rPSi} is the relative permittivity of PS, ϵO is relative permittivity of vacuum, μ_{eff} is the mobility of charge carriers , and V is the voltage The relative permittivity of the PS is proportional to the Porosity(%) of the PS layer[13]. The relative permittivity ($\epsilon_{r\ PSi}$) and hence the refractive index(n_{PSi}) of PS is a function of the morphology properties especially the type of gas inside the PS channels and the Porosity(%)of PS. The relative permittivity of Si substrate is about ($\epsilon_{r\ Si}$=11.6) while the $\epsilon_{r\ PSi}$ was determined from equation (5). Generally it can be seen from Figure-7 that the relative permittivity ($\epsilon_{r\ PSi}$) in the present air andCO_2gas filled PSi layer decreases with increasing the etching time. The relative permittivity of PS layer in the present air is different from the value of silicon .This means the PS is a new material with new properties Which is define as the mixture between two material pores channels and silicon (Si) material. Increasing the etching mechanism can explain the decrease in the relative permittivity and hence the increase of void space (air) and decrease of the silicon skeleton in porous matrix [14] .

$$\epsilon_{r\ PSi} = (1\text{-}P\%)\, \epsilon_{Si}^{1/3} + P\%\epsilon_{air}^{1/3} \quad \text{…………………(5)}$$

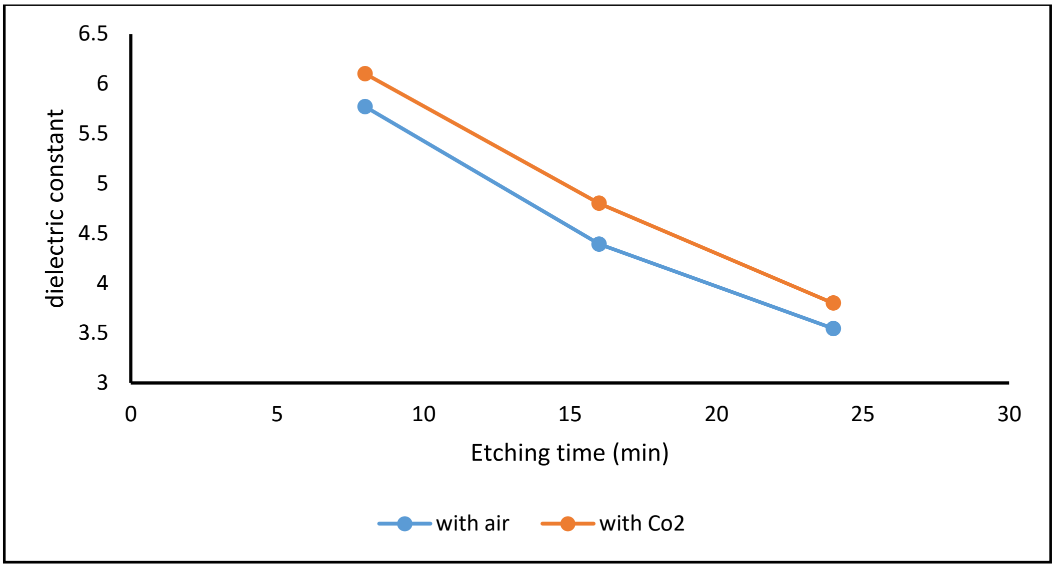


Figure 7-The relative permittivity as a function of the etching time with air and with Co_2 gas.

The condensation process occurred in the silicon channels because of the thermal conductivity.When the pores channels become very small, they behave as thermal insulator and the Porosity (%) is high. This change in the relative permittivity of the PS matrix will modify all the electric and also the gas sensing properties. Figure-8 show the current density as a function to etching time according to equation (4).

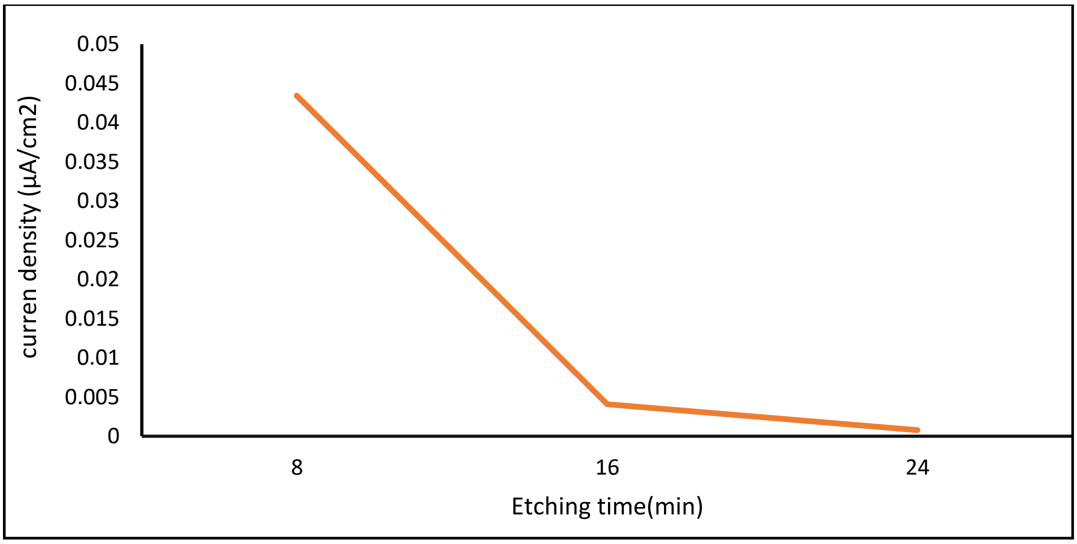


Figure 8-The relation between the current density and etching time

Conclusion

This research study the formation of porous silicon gas sensor on silicon wafer at different etching times and measuring the J-V characteristic using a homemade gas sensor device .The results are as shown in Figure-6.The current density waes determined using equation(4) using MATLAB program as shown in Figure-8. In each figure the current density decreases with the increase of etching time.Thus the change in the current density is due to the rearrangement of charge carriers and presents traps on the porous silicon surface. This is controlled by the depletion layer inside PSi rather than the hetrojunction between PS/Si. From the resultsit can be seen that the electrical properties of PSis change according to the layer thickness, when the layer thickness is relatively small of about (1µm) the electrical properties are different from those of the thick layer.The current flow for thin PSi Layer thickness (%) was due to PSi/Si hetrojunction within the metal /PSi/Si structure.

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