Calculation of Energy Band gap of Porous Silicon Based On The Carrier Transport Mechanisms

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Abstract

The energy bandgap of photoluminescence porous silicon is calculated based on the analysis of the current-voltage characteristics and the measurements of the thermal activation energy of the zero bias and reverse bias currents of PS/n-Si porous silicon diodes at different temperatures. The 2.1 eV bandgap resulting from these electrical measurements agrees well with 2 eV measured in PL spectra.

حساب فجوة الطاقة للسليكون المسامي بالأعتماد على آلية أنتقال الشحنة

الخلاصة

في هذا البحث تم حساب فجوة الطاقة للسليكون المسامي المتلألأ بالأعتماد على تحليل خصائص التيار - الفولطية وقياس طاقة التنشيط الحراري عند جهد (0V) وتيار الأنحياز العكسي لديودات (PS/n-Si) عند درجات الحرارة المختلفة.
أن فجوة الطاقة المقاسة كانت2.1eV بالأعتماد على القياسات الكهربائية وتتفق مع القيمة المقاسة بالأعتماد على خصائص (PL) البالغة (2eV)

1. Introduction

Porous silicon (PS) has been identified as a potential optoelectronic material compatible with silicon technology after the discovery of strong room-temperature photoluminescence (PL) from high porosity PS in 1990 [1]. Electroluminescence (EL) is also observed from Schottky diodes formed from PS [2]. The bandgap of PS was determined upon the peak of the PL and EL spectra [3, 4]. The study of the transport mechanisms of charge carrier plays an important role in development of PS-based devices such as light emitting devices, photodetectors, solar cells, etc [5, 6]. The analysis of carrier transport mechanism in PS to determine the bandgap of the PS was firstly done by Chen *et al*. [7] in homojunction p-n porous silicon diodes. Timikhov *et al*. [8], have studied the evaluation of bandgap of PS using the photoelectric properties (i.e. photocurrent of PS/p-Si heterojunction under different

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exciting photon energy sources 1.5-3.5 eV with constant intensity).
The present investigation reports the calculation of energy bandgap of photosynthesis porous silicon based on the current-voltage characteristics of PS/n-Si heterostructure.

2. Experiment

The self-formation of PS/Si heterojunction was achieved by photochemical etching process of silicon substrate of resistivity 4.3-5.6 cm in hydrofluoric acid with 50 minutes etching time. More details of this process can be found elsewhere [9, 10]. The PS/n-Si heterojunction was made with 74% porosity and 25 m thick of the PS layer. The value of the mean porosity over the thickness of PS layer and the thickness of PS layer were determined gravimetrically. The electrical measurements of PS/Si heterodiodes were carried out using fine power supply and digital electrometers. Photoluminescence measurement was done by using He-Cd laser at a wavelength of 325 nm with a low laser power density of nearly 10 mW/cm^2.

3. Results and Discussion

The photosynthesized PS layer exhibited appreciable photoluminescence as shown in Fig. (1) with peak PL at 2.0 eV corresponds to the bandgap of the synthesized PS.
The peak PL of PS is greatly affected by the porosity. For PS layer of > 80% porosity shows a green-blue to blue peak emission, otherwise it should exhibit a red peak emission. In our case, the PL peak shows red emission (620 nm) which is in consistent with the measured porosity

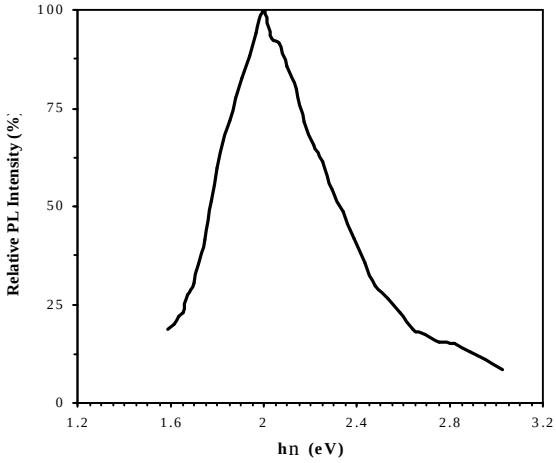

Fig. (1). Spectral PL of the photosynthesized PS.

It is recognized previously that PS formed from p-type is n-type and that produced from p-type is n-type [6], therefore PS/n-Si heterojunction is thought to be isotype heterojunction. DC measurements were made in dark on a number of PS/Si samples for temperature range between 300 K and 380 K. The deviation of IV characteristics for thick porous layer from the ideal one is due to
the existence of series resistance (R_S). Forward IV dependence therefore is analogous to that of diode with series switched resistance [5, 11].

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

(1)

Where I_S is the saturation current obtained from semi-log forwarded bias, k, T and q have their usual meaning.

Series resistance is voltage dependent. It is also depends on the thickness and porosity of the PS layer [5], therefore the determination of saturation current value from extrapolating the measured forward bias IV curve is not quite credit prove and shows difficulties to determine by several workers. We therefore measured the saturation current directly under reverse bias conditions beside the extrapolated saturation current at zero bias to assure the validity of the results. The measurements of the saturation current under reverse bias voltage were carried out at different reverse bias voltages and temperatures and plotted in semi-log graphs as shown in Fig. (2). This figure clearly shows that the measured data can be well approximated by a straight-line region.

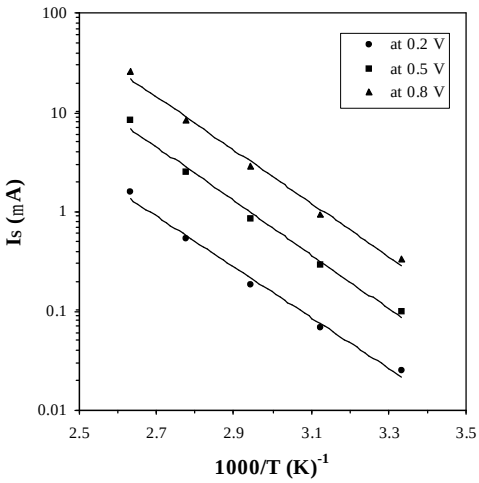

Fig. (2) Semi-log I_S against reciprocal of temperature.

The thermal activation energies calculated from the slope of $\ln I_S$ versus T^{-1} are listed in Table (I). The linear behavior of $\ln I_S$ versus T^{-1} indicates the domination of one component of the diode reverse current, where the diode reverse current is divided into four components according to the location of carrier recombination and generation [7, 12-14]. They are respectively:

1. Bulk diffusion current (I_{bd}) given by:

$$I_{bd} = I_{bds}\left[\exp\left(\frac{qV}{kT}\right) - 1\right] \quad (2)$$

with $I_{bds} \sim n_i^2$

2. Bulk recombination-generation current (I_{br}) stemming from carrier recombination and generation in depletion region between bulk n-Si and PS region:

$$I_{br} = I_{brs}\exp\left(\frac{qV}{2kT}\right) \quad (3)$$

with $I_{brs} \sim n_i$

3. Surface recombination-generation current (I_{sr}) caused by the recombination and generation of carriers at the surface of the junction:

$$I_{sr} = I_{srs}\exp\left(\frac{qV}{2kT}\right) \quad (4)$$

with $I_{srs} \sim n_i$

4. Surface channel current (I_{sc}) results from the recombination and generation of carriers in the depletion region formed between the surface channel and n-type bulk silicon:

$$I_{sc} = I_{scs} \exp\left[\left(\frac{qV}{2kT}\right) - 1\right]^{1/2} \quad (5)$$

with $I_{sc} \sim n_i^{1/2}$

The prefactors I_{bds}, I_{brs}, I_{srs}, I_{scs} are the saturation current respectively. The saturation current implicitly depends on temperature via the intrinsic carrier density (n_i), where for silicon quantum wire the dependence of n_i on the temperature is given by:

$$n_i \approx T \exp \frac{-Eg}{kT} \quad (6)$$

Table (I). Activation energy (E_a) calculated from $\ln(I_S)$-T^{-1}.

Bias Voltage (V)	E_a (eV)
0.2	0.507
0.5	0.540
0.8	0.530

In diodes such as our porous silicon diodes, we believe that the most important component that will contribute to the total reverse current is the surface channel reverse current, I_{srs}. This belief is based on the following reasons.

1- Since the fabricated porous silicon diodes are not electrically passivated, the generation and recombination of charge carrier in the space-charge region of surface channel is the main contributor to the reverse bias saturation current.

2- The high value of the ideality factor (m) that is calculated from Fig. (3) and illustrated in Fig. (4) proves that the surface channel is present in our diodes [5, 7,14].

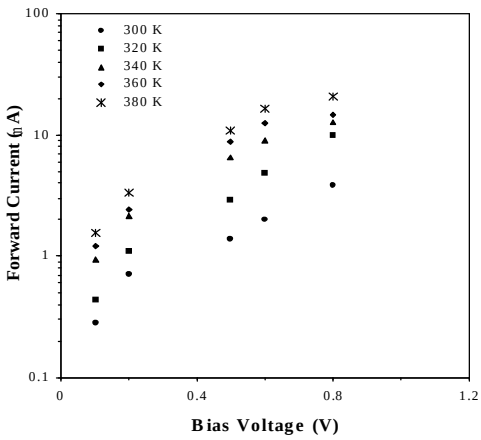

Fig. (3). IV characteristics of PS/Si

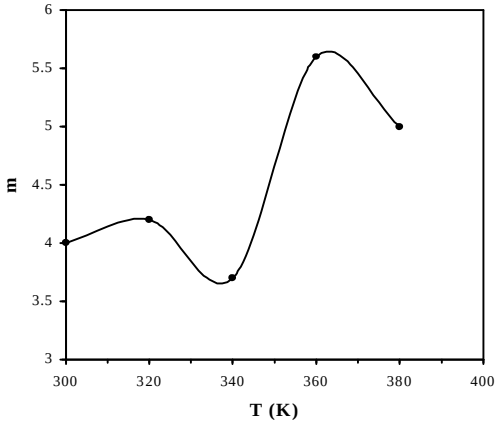

Fig. (4). Ideality factor as function of temperature.

3- The feature size of PL active porous silicon is in the nanometer range. The specific surface is very high (about 600 m^2/cm^3), these will lead to the fact that the surface effect in porous silicon diodes is very important, as a result, the surface channel current component is expected to play important role in porous silicon diodes. This current is more important particularly for PS diodes with thick PS layer [5]. For PS diodes with thin porous layer, the reverse current is determined by the generation and recombination of carriers in the depletion region of crystalline silicon, with ideality factor close to 2 and activation energy equal half of the crystalline silicon (about 0.58 eV).

The saturation current associated with the surface channel component is described by equation (5). Since the current is proportional to $n_i^{1/2}$, its measured thermal energy is thus one fourth of energy gap of silicon nanowire[7]. Therefore, the measured bandgap for PS diodes is 2.1 eV, i.e, four times of the average activation energy of 0.525 eV. This result is in fair agreement with that of PL result.

Fig. (5) depicts the exponent relation between extrapolated I_S from zero bias voltage and T^{-1}. The bandgap calculated from this method is 2.11 eV with in good coincidence with the results of Fig. (2). This agreement indicates the validity of this method in calculating bandgap and contradicts with results of ref. [5]. The precise determination of the linear region of the semi-log IV curve can make this method more precise and can give consistent results obtained to other methods.

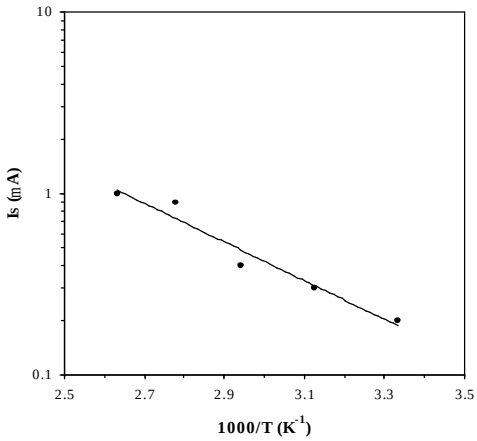

Fig. (5). Relationship between I_S and T^{-1}.

4. Conclusions

Al/PS/n-Si/Al porous silicon diodes resulting from thick porous layer have forward and reverse current-voltage characteristics depend strongly on the surface channel current. The measured thermal activation energy of the reverse saturation current indicates that the electrical bandgap changes from 1.12 eV for bulk crystalline silicon to 2.1 eV for photosynthesized porous silicon.

The measured 2.1 eV bandgap resulting from these electrical measurements agrees well with 2 eV bandgap measured from PL measurements.

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