1. Introduction

Porous silicon (PS) is a special composite material consisting of pores and silicon backbone networks. It has a broad range of applications due to its high ratio of surface atoms that determine the high tunability of the PS in many properties such as dielectric constant [1,2], band gap [3] and chemical reactivity [4,5].

According to the model proposed by Canham [6,7], the recombination of electron–hole pairs occurs within nanometer silicon wires and their energy gaps become larger than that of bulk Si (quantum confinement effect). This model, modified by Koch et al. [8], suggests that electron–hole pairs are photo-excited in nanometer silicon particles and recombined via Si intrinsic surface states.

Several models have been proposed for studying the transport of carriers in PS based metal/PS/c-Si device structures [9–13]. To explain the experimental results, these models assume either that the reverse current is determined by the surface transport mechanism of hopping [11], or with carrier generation in surface states at the boundary between Porous silicon and c-Si substrate [10]. It was found that the forward current–voltage (I–V) dependence exhibits a relatively short exponential region with a quality factor of 4 or higher [10–13]. Pan et al. [14] have developed a method to characterize the dielectric properties of PS as a function of its porosity and the surface oxidation that are adjustable to experiment.

Besides, Milani et al. [15] have surveyed optoelectronic effects in PS using experimental measurements of photoluminescence (PL), current–voltage, surface resistance and specular reflectance of PS samples prepared with increasing etching time. These measurements have clarified the relationship between the observed behavior and porosity, and showed an increase of the band gap from 1.83 to 2 eV.

Porous materials are used in many areas of applied science and engineering and have taxonomies based on different criteria such as pore size, pore shape, materials and production types. Cicke and Celik [16] have proposed a decision aid mechanism based on fuzzy axiomatic design (FAD) to select adequate form of porous materials in marine systems design, and they addressed use of porous materials in plate type heat exchanger design to demonstrate the proposed model. Edwards [17] had chosen the optimal material and manufacturing process combination that regards a novel idea. Besides the feasible applications of this approach in engineering component design, the increasing complexity of technical system (i.e. energy plant, offshore, etc.) requires great potential, and the material selection of components is one of the most challenging issues in the design and development of technical systems. Furthermore, various studies have been performed to help address the issue of material selection. There are few methodological approaches towards solution of the problem as fuzzy knowledge based decision support system [18].

Although there were reviews which have been published throughout the past years, there exists no detailed study...
adequately documenting the optical properties using specific models, the structural properties, elastic properties and Debye temperature parameters as a function of porosity. This is due to the large number of the independent parameters (energy gap, bulk modulus, elastic constants and shear modulus), the chemistry and pore formation mechanisms that remain largely unknown. Refractive index, optical dielectric constant, bulk modulus, elastic constants and short-range force constants are investigated. Also, shear modulus, Young’s modulus, Poisson’s ratio and Lame’s constants for both bulk Si and PS are derived. The Debye temperature of PS is estimated from the average sound velocity. Additionally, the optical properties and elasticity of PS are reported for the first time estimated from the average sound velocity. Additionally, the optical properties and elasticity of PS are reported for the first time.

The paper is organized as follows. In the following section the computational method is used in the present work. Section 3 is devoted to the presentation of our results comparing with previous calculations and experimental studies. A conclusion of the present work is given in Section 4.

2. Computational method

Using the Empirical Pseudopotential Method (EPM), the symmetric and antisymmetric pseudopotential form factors have been adjusted in order to fit the experimental energy band gaps of bulk and PS which are given in Table 1. Adjustments to the specific pseudopotential form factors are made using a nonlinear least-squares [21] fitting procedure. The lattice constant used for the bulk Si is 5.431 Å. The final adjusted symmetric and antisymmetric pseudopotential form factors have been adjusted in order to fit the experimental energy band gaps of bulk Si and PS which are given in Table 1. Adjustments to the specific pseudopotential form factors have been adjusted in order to fit the experimental energy band gaps of bulk Si and PS which are given in Table 1. Adjustments to the specific pseudopotential form factors have been adjusted in order to fit the experimental energy band gaps of bulk Si and PS which are given in Table 1. 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electronic properties. Knowledge of the refractive index is essential for devices such as photonic crystals, wave guides, solar cells and detectors [24]. On the other hand, n is closely related to the energy band structure of the material. Consequently, many attempts have been made in order to relate the refractive index and the energy gap of the material. Consequently, many attempts have been made in order to relate the refractive index and the energy gap through simple relationships [25–30]. However, these relations of the percentage porosity. Thus, these three models of variation of n with energy gap have been calculated. Our results for PS are compared with experimental and theoretical data in the literature. Our result concerning B0 for bulk Si is in good agreement with the experimental one reported in Ref. [40]. Moreover, it agrees very well with the theoretical calculations [41,42]. The variation of B0 as a function of porosity is plotted in Fig. 3. Note that as the percentage porosity increases, B0 decreases gradually. The

\[
B_0 = (30 + 10 \beta)(P_1^{1/2}/E_{Gf-X})/3
\]  

where \(P_1\) is the transition pressure, \(E_{Gf-X}\) is the energy gap along \(\Gamma - X\) and \(\beta\) is a parameter appropriate for the group-IV = 0, III–V = 1 and II–VI = 5 semiconductors. Our results of B0 are listed in Table 3 along with the experimental and theoretical data in the literature. Our result concerning B0 for bulk Si is in good agreement with the experimental one reported in Ref. [40]. Moreover, it agrees very well with the theoretical calculations [41,42]. The variation of B0 as a function of porosity is plotted in Fig. 3. Note that as the percentage porosity increases, B0 decreases gradually. The

\[
C_{11} (10^{11} \text{ dyn/cm}^2), C_{12} (10^{11} \text{ dyn/cm}^2), C_{44} (10^{11} \text{ dyn/cm}^2), \alpha (N/M), \beta (N/m)
\]

Table 3

<table>
<thead>
<tr>
<th>Porous silicon (%)</th>
<th>Bulk modulus B0 (GPa)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Cal.</td>
</tr>
<tr>
<td>0</td>
<td>100.7</td>
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<tr>
<td>27</td>
<td>97.85</td>
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<td>77.10</td>
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<td>43</td>
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<td>73</td>
<td>62.11</td>
</tr>
<tr>
<td>75</td>
<td>60.43</td>
</tr>
<tr>
<td>88</td>
<td>59.46</td>
</tr>
</tbody>
</table>

Cal. Exp.\textsuperscript{a}:

\[
0 17.9 16.57 7.71 6.39 8.16 7.96 55.71 48.50 13.84 13.81
27 56.5 – 2.42 – 2.58 – 22.10 – 5.53 –
33 4.74 – 2.03 – 2.71 – 19.20 – 4.80 –
43 3.29 – 1.41 – 1.50 – 14.34 – 3.59 –
58 2.99 – 1.28 – 1.37 – 13.28 – 3.32 –
65 1.70 – 0.73 – 0.78 – 8.47 – 2.11 –
73 1.61 – 0.69 – 0.74 – 8.10 – 2.02 –
75 1.40 – 0.60 – 0.64 – 7.24 – 1.81 –
88 1.29 – 0.55 – 0.59 – 6.76 – 1.70 –
\]

\textsuperscript{a} Ref. [40] exp.
\textsuperscript{b} Ref. [41].
\textsuperscript{c} Ref. [42].
\textsuperscript{d} Ref. [43].

Table 2

<table>
<thead>
<tr>
<th>Porous silicon (%)</th>
<th>Calculated refractive indices (n) and high-frequency optical dielectric constant ((\varepsilon_{\infty})) for bulk Si and PS using: Ravindra et al. [30], Herve and Vandamme [31] and Ghosh et al. [32] models.</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Porosity (%)</td>
</tr>
<tr>
<td>0</td>
<td>3.395\textsuperscript{a}, 3.177\textsuperscript{b}, 3.432\textsuperscript{c}, 11.520\textsuperscript{a}, 10.939\textsuperscript{b}, 11.778\textsuperscript{c}</td>
</tr>
<tr>
<td>27</td>
<td>3.216\textsuperscript{a}, 3.004\textsuperscript{b}, 3.202\textsuperscript{c}</td>
</tr>
<tr>
<td>33</td>
<td>3.185\textsuperscript{a}, 2.977\textsuperscript{b}, 3.162\textsuperscript{c}</td>
</tr>
<tr>
<td>43</td>
<td>3.116\textsuperscript{a}, 2.918\textsuperscript{b}, 3.078\textsuperscript{c}</td>
</tr>
<tr>
<td>58</td>
<td>3.098\textsuperscript{a}, 2.903\textsuperscript{b}, 3.056\textsuperscript{c}</td>
</tr>
<tr>
<td>65</td>
<td>2.98\textsuperscript{a}, 2.809\textsuperscript{b}, 2.927\textsuperscript{c}</td>
</tr>
<tr>
<td>73</td>
<td>2.968\textsuperscript{a}, 2.83\textsuperscript{b}, 2.914\textsuperscript{c}</td>
</tr>
<tr>
<td>75</td>
<td>2.937\textsuperscript{a}, 2.776\textsuperscript{b}, 2.883\textsuperscript{c}</td>
</tr>
<tr>
<td>88</td>
<td>2.918\textsuperscript{a}, 2.763\textsuperscript{b}, 2.864\textsuperscript{c}</td>
</tr>
</tbody>
</table>

\textsuperscript{a} Ref. [30].
\textsuperscript{b} Ref. [31].
\textsuperscript{c} Ref. [32].
\textsuperscript{d} Ref. [35,36] exp.
\textsuperscript{e} Ref. [37] exp.

Fig. 2. Variation of refractive index versus porosity percentage for Porous silicon (PS), using different models.
We now turn our attention to the elastic properties. In this respect, the elastic constants namely $C_{11}$, $C_{12}$ and $C_{44}$ have been calculated following the same procedure used by Bouarissa [44] that was based essentially on the work of Baranowski [45], where $C_{11}$, $C_{12}$ and $C_{44}$ are expressed as,

$$C_{11} = \frac{\sqrt{3}h}{4d^2m}(1 - \alpha^2)^{3/4}[4.37(5 + \lambda)(1 - \alpha^2) - 0.6075]$$  \hspace{1cm} (10)

$$C_{12} = \frac{\sqrt{3}h}{4d^2m}(1 - \alpha^2)^{3/4}[4.37(3 - \lambda)(1 - \alpha^2) + 0.6075]$$  \hspace{1cm} (11)

$$C_{44} = \frac{3}{4d^4}(\alpha + \beta - 0.1365C_0 - C_0^2)$$  \hspace{1cm} (12)

In Eqs. (10)-(12), $d$ is the nearest neighbor distance, $\lambda$ is a dimensionless parameter which has a constant value of 0.738 [45] and $l$ is the electron mass. The quantities $\alpha$ and $\beta$ in Eq. (12) are the short-range force constants. They represent the bond-stretching and bond-bending force constants, respectively and are expressed as [46],

$$\alpha = \frac{d}{\sqrt{3}}(C_{11} + 3C_{12}) + \frac{d}{3\sqrt{3}}(1.473SC_0)$$  \hspace{1cm} (13)

$$\beta = \frac{d}{\sqrt{3}}[(C_{11} - C_{12}) - 0.0535C_0]$$  \hspace{1cm} (14)

The parameter $\xi$ is the internal-strain parameter. The quantities $S$ and $C_0$ are obtained using the following expressions,

$$S = \frac{Z^2}{\varepsilon(0)}$$  \hspace{1cm} (15)

$$C_0 = \frac{e^2}{d^4}$$  \hspace{1cm} (16)

$S$ is an effective charge parameter, $C_0$ has the dimensions of an elastic constant and $\varepsilon$ is the effective charge. More details about the determination of the quantities $C$, $\zeta$ and $\varepsilon$ are given in Ref. [46]. $\varepsilon(0)$ is the static dielectric constant.

Our results concerning $C_{11}$, $C_{12}$ and $C_{44}$ for bulk Si and PS are given in Table 3 including the experimental and theoretical data for comparison. Generally, our results agree reasonably well with those reported in the literature.

The variation of the elastic constants $C_{11}$, $C_{12}$ and $C_{44}$ as a function of the porosity is displayed in Fig. 4. One can observe that all the studied elastic constants decrease non-linearly with increasing the porosity. However, it should be noted that the following behavior is seen. Qualitatively, the trends of elastic constants of PS are similar. From the quantitative point of view, the elastic constants show considerable differences according to the porosity changes, where they have larger values when Si has low porosity and smaller values when Si has high porosity on the entire range of porosity.

The calculated bond-stretching and bond-bending force constants as well as the internal-strain parameter for the bulk Si and PS with available data in the literature are shown in Table 3. From Table 3, one can see that our results agree well with those obtained experimentally [40,43]. For PS, the quantities $\alpha$ and $\beta$ are seen to have larger values when PS has low porosity and smaller values when PS has high porosity.

The variation of the bond-stretching and bond-bending force constants as a function of the porosity are plotted in Fig. 5. According to this figure, one can see that increasing the porosity leads to a decrease of both force constants. This trend is almost similar to those shown by the elastic constants that imply the PS could provide more opportunities to obtain desired elastic and short-range force constants with changing the porosity percentage.

Having calculated the Young's modulus $E$, bulk modulus $B_0$ and shear modulus $G$, one can calculate the Debye temperature, which is an important fundamental parameter closely related to many physical properties such as elastic constants, specific heat and...
melting temperature. We have estimated the Debye temperature \( \theta_D \) of bulk Si and PS from the average sound velocity, \( v_m \), by the following equation [47]:

\[
\theta_D = \frac{h}{k_B} \left( \frac{3}{4\pi V_a} \right)^{1/3} v_m
\]  

(17)

where \( h \) is the Planck’s constant, \( k_B \) the Boltzmann’s constant and \( V_a \) is the atomic volume. The average sound velocity in the polycrystalline material is given by:

\[
v_m = \frac{1}{\sqrt{\frac{1}{v_l^2} + \frac{1}{v_t^2}}} \]  

(18)

where \( v_l \) and \( v_t \) are the longitudinal and transverse sound velocity obtained using the shear modulus \( G \) and the bulk modulus \( B_0 \) from Navier’s equation [47]:

\[
\frac{1}{3} \left( \frac{3B + 4G}{3G} \right)^{1/2} \quad \text{and} \quad \frac{1}{v_l} = \left( \frac{G}{\rho} \right)^{1/2}
\]

(19)

The calculated sound velocity and Debye temperature as well as the density for PS are given in Table 4. It is shown that our calculated results of 0% PS are in good accordance with experimental values [48–54]. For PS, the correlation of the calculated values with porosity is proportional inversely. Future works will test our calculated results. The present results stand, therefore, as reliable predictions for these parameters.

4. Conclusions

Increasing the band gap of Porous silicon (PS) with porosity is proportional inversely. Future works will test our calculations for energetic transitions and elastic properties are obtained. The sound velocity and Debye temperature are estimated and showed a good accordance with experimental results.

Acknowledgment

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References
