Structural, Electronic and Optical Properties of 6H-SiC and 3C-SiC with the Application in Solar Cell Devices

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Abstract. 6H-SiC and 3C-SiC structural, electronic and optical properties have been calculated by applying the principles of density functional theory based on the plane wave pseudo-potential. This method is implanted in Wien2k Software. Structural parameters are calculated at the level of Perdew Burke and Ernzerhof (PBE) parameterized generalized gradient approximation (GGA). The obtained results given in Table I were compared to the experimental data in relation with the lattice constant hexagonal ration c/a and the band gap value parameters of 6H-SiC and 3C-SiC, there was a very accurate concordance.

The superior gap value and the good absorption coefficient drives us to realize a p⁺nn⁺ solar cell device using SILVACO Software. The 3C-SiC material resulted in a considerable performance for photovoltaic applications.

Introduction

The SiC semiconductor as a excellent promising material for solar cells and electronic application, mainly for their high band gap, good chemical resistance and thermal conductivity [1,2]. Record conversion efficiency up to 17.86% has been reported in single-junction 3C-SiC solar cells with 5µm thickness, and 26.09% for 3C-SiC/Si tandem structure [3]. This present work proposes PIN structure based on 3C-SiC Solar cells to calculate the current–voltage (J–V) characteristics and the internal quantum efficiency (IQE (λ)).

Many authors investigated the SiC solar cells devices, Noor Alhuda et al., [4] have studied the Influence of Environmental Factors on the Performance of 3C-SiC PIN structure Solar Cells. They obtained 30.27 % Record conversion efficiency under 1000W.m⁻² Light intensity. The studies led by [5] single-junction solar cells based on 3C–SiC material evaluated using a two-dimensional finite element method. The efficiencies of 12.52% is obtained for 0.2 μm of n + and p + thicknesses. Hamid Heidarzadeh et al. [6] they found an optimal efficiency for 3C-SiC achieved in 55.9% under a 1000 suns concentration and AM1.5 spectrum irradiation. This work investigates 6H-SiC and 3C-SiC structural, electronic and optical properties with solar cell devices application. we can organize as follows; the first section focuses on 6H-SiC structural, electronic, and optical properties results within the density functional theory. The second section 3C-SiC PIN solar cells structure proposed, to calculate photovoltaic parameters.

The First Section

Computational methods. The functional density theory within the plane wave pseudo-potential approach as implemented in the WIEN2 code to calculate structural, electronic and optical properties, the Kohnsham equation were solved using (PBE-GGA) for the exchange correlation energy. Throughout our calculation $R_{mt} \bullet K_{max} = 9.5$ is taken, where R_{mt} represents the smallest muffin tin radius of atoms ($S_i = 1.62$ and $C = 1.71$), K_{max} is the maximum value to the reciprocal

lattice vector used in the plane wave expansion. The potential and the charge density were Fourier expanded up to $G_{max} = 12$.

Structural, Band structure and optical properties. The crystal structure of 6H-SiC and 3C-SiC is hexagonal with space group P63mc (186). The Si atoms are located in 2b Wyckoff site with fractional coordinates (1/3,2/3,3/8), and the C atoms are situated in 2b Wyckoff site with fractional coordinates (1/3,2/3,3/8). The total energy has been calculated and minimized of 6H-SiC and 3C-SiC to different cell volumes, Fig. 1 and Fig. 2 respectivly. The obtained results given in Table I were compared with results data reported in Reference [7,8] in relation with band gap , the lattice constant and hexagonal ratio c/a.
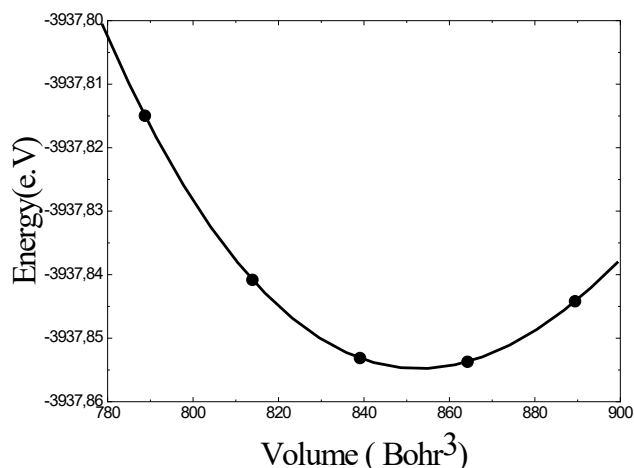

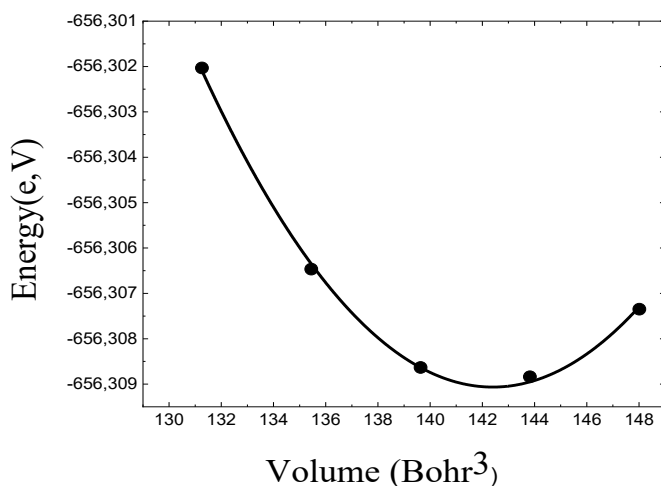Fig 1. Total energies as a function of volume of 6H-SiC.

Fig 2. Total energies as a function of volume of 3C-SiC.

Table I. The Lattice constant, hexagonal ration c/a and band gap of 6H-SiC and 3C-SiC.

	Eg(eV)	Structure		
		a(A)	c(A)	c/a
6H-SiC Present work	2.015	3.0817	15.1179	4.9057
6H-SiC Reference[5]	2.01	3.0806	15.117	4.9071
3C-SiC Present work	1.37	4.384	-	-
3C-SiC Reference[6]	2.42	4.36	-	-

The 6H-SiC and 3C-SiC band structure is presented in Fig. 3 and Fig. 4. It is clear that the 6H-SiC has a indirect band gap with the valence band maximum at G-point and the conduction band minimum locates at the M-point. Also 3C-SiC has an indirect band gap with the valence band maximum at X- point and the conduction band minimum locates at the G-point, the calculated band gap for 6H-SiC and 3C-SiC are 2.015 eV and 1.37 eV respectively.
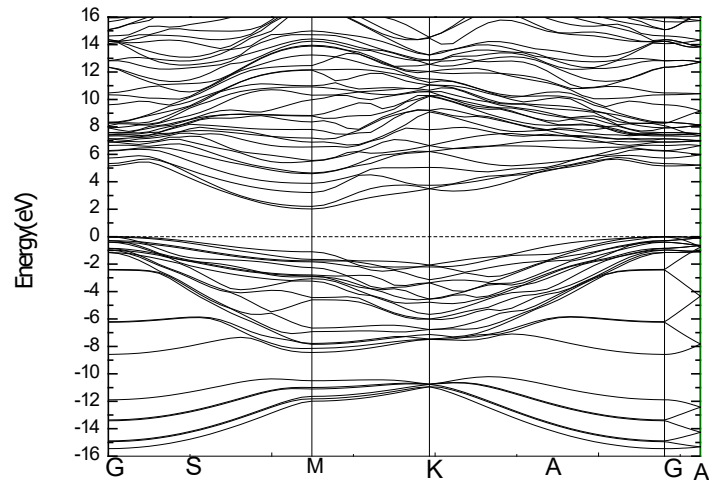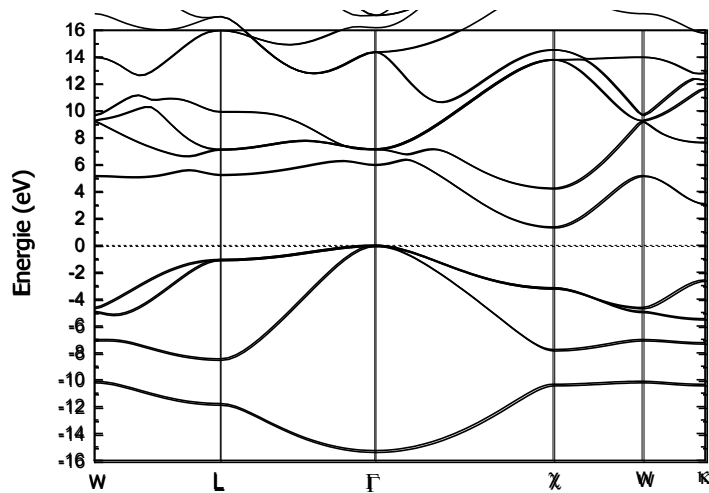

Fig 3. Band structure of 6H-SiC.
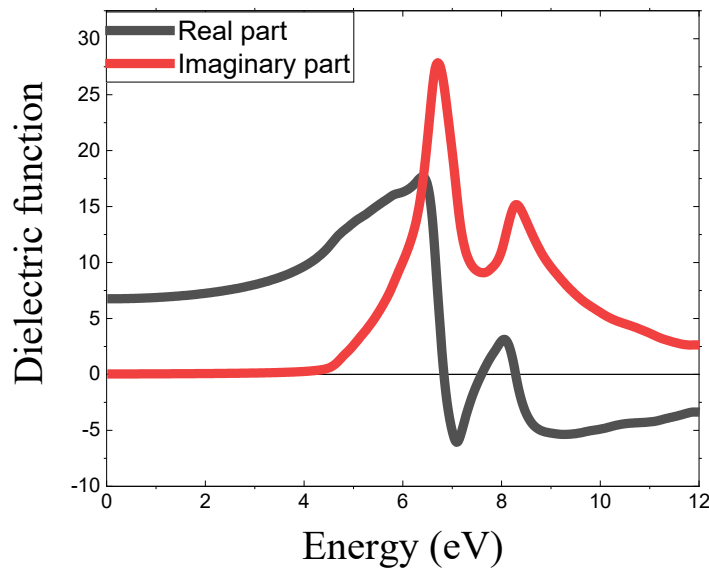

Fig 4. Band structure of 3C-SiC.
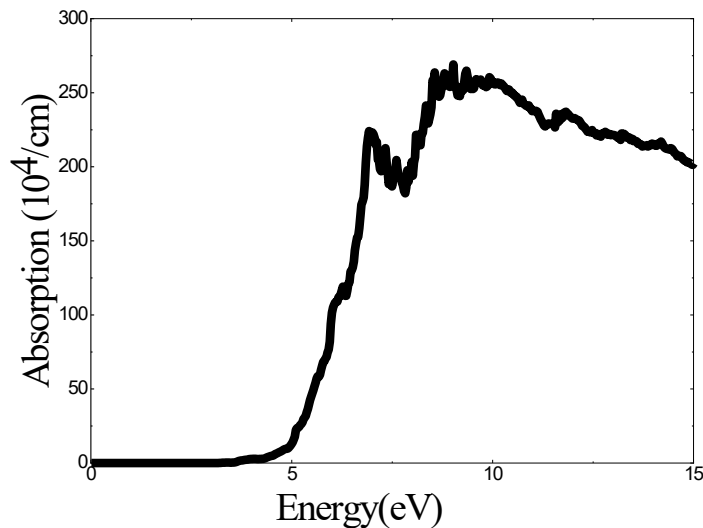
Fig 5. The dielectric function of 6H-SiC.

Fig 6. The absorption coefficient of 3C-SiC.

Fig. 5 shows dielectric function of 3C-SiC in theoretical calculation, in which the imaginary part of dielectric function contains high-energy zone from 5 to 12 eV, the imaginary part of dielectric function increases rapidly from 6.25 eV with dielectric peaks at 27.5 then decreases with the increase of energy as result the decreases of optical absorption of inter-band electron transition in Fig .6, the same behavior has been reported in Ref. [6]. We can show that the 3C-SiC is a good choice in solar cells application.

The Second Section

The obtained results in the first section prompted us to study PIN solar cells based on 3C-SiC, the simulation have been carried out using ATLAS SILVACO software for the solution of two dimension, Poisson equation and the continuity equations for free charge carriers.

$$\varepsilon \Delta V = \text{-q } (p - n + N_D - N_A). \tag{1}$$

$$\nabla(n\mu_n E + D_n \nabla n) = 0. \tag{2}$$

$$\nabla(n\mu_n E + D_n \nabla n) = 0 \tag{3}$$

Where V is the electrical potential, ε is the permittivity, q is the elementary charge, p,n are the hole, electron concentrations respectively, N_D, N_A the density of ionized acceptors and donors respectively. μ_n and n μ_p are the electron and hole mobility. D_n and D_p are the electron and hole diffusion coefficient. R is the (SRH) recombination rate of free electrons and holes. The parameters used in the simulation are listed in Table 2. The solar cell is assumed to be operating under standard conditions, AM1.5 illumination spectrum and temperature T = 300 K. Fig. 7 and Fig. 8 shows the simulated current-voltage (J-V) characteristic and external quantum efficiency (EQE).

Table 2. Parameters used in the simulation at T=300 K.

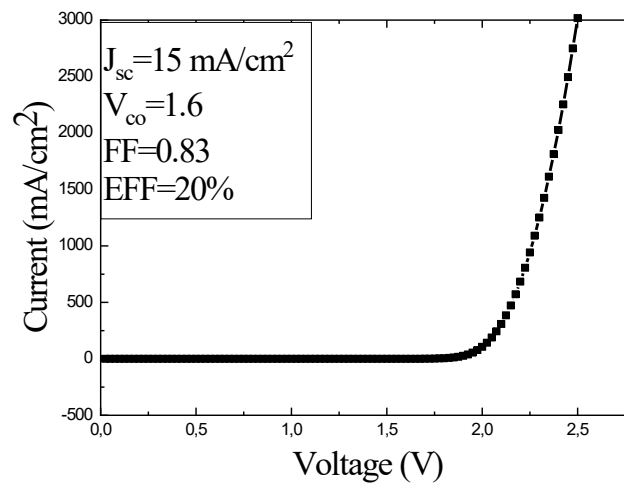| Parameter	Symbol	Value	Unit
band gap	E_g	3.02	eV
electron affinity	χ	3.6	eV
effective density of states	N_c ,N_v	2.10^{18}	cm^{-3}
electron mobility	μ_n	100	$cm^2/V.s$
hole mobility	μ_p	320	$cm^2/V.s$
dielectric constant	ε	4.9	
Electron life time	$\tau(n)$	30	$\mu(s)$
Hole life time	$\tau(p)$	10	$\mu(s)$

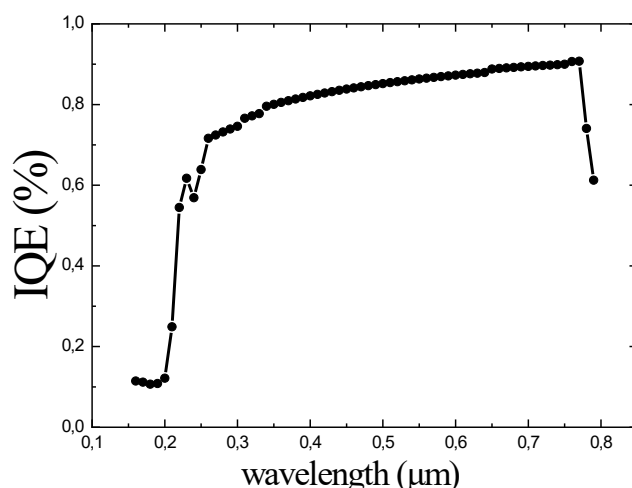Fig 7. Current density–voltage characteristic (J-V) of 3C-SiC solar cells.

Fig 8. Internal quantum efficiency (IQE) of 3C-SiC solar cells.

Summary

This paper investigated the solid state properties such as structural, electronic and optical properties of 6H-SiC and 3C-SiC, using the first-principles calculation. Our simulations show that 3C-SIC is a good choice for photovoltaic applications.

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