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Effects of emitter parameters and recombination mechanisms on the performance of β-$FeSi_2$/c-Si heterojunction solar cells

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ABSTRACT

In this paper, numerical simulations on the performance of p-type β-$FeSi_2$ emitter/n-type crystalline Si base heterojunction solar cells are carried out using PC1D software. The dependences of performance on layer thickness and doping concentration in the emitter region are analyzed. The influences of main recombination mechanisms in the emitter region for cell characterization are discussed. The simulation results show that both emitter thickness and doping concentration have very important influences on the property of β-$FeSi_2$/c-Si heterojunction solar cells. These two parameters need to be jointly selected to improve cell performance. The optimal values of emitter thickness and doping concentration are 350 nm and 2×10^{17} cm^{-3} for the cell structure, respectively. Moreover, cell efficiency can be enhanced by suppressing carrier recombination rate. Bulk and surface recombinations must be minimized by improving the material growth and surface passivation process, and the Auger and radiative recombination can be suppressed by reducing carrier concentrations appropriately. With the emitter parameter optimized, device performance can be well improved.

1. Introduction

Semiconducting iron disilicide (β-$FeSi_2$) is an attractive material due to its remarkable optical properties such as a direct band gap of 0.87 eV and very large optical absorption coefficient ($\alpha > 10^5$ cm^{-1}) [1–7]. β-$FeSi_2$ also possesses fairly good compatibility with the Si-process technology. Moreover, β-$FeSi_2$ is considered to be an environmentally friendly semiconductor since both Si and Fe are nontoxic and in great abundance on earth. Therefore, β-$FeSi_2$ is a new promising candidate for optoelectronic and photovoltaic applications [8–10].

Recently, heterojunction solar cells with β-$FeSi_2$ thin films deposited on crystalline silicon (c-Si) wafers for photovoltaic application were fabricated by several groups [11–16]. However, their reports indicated the highest conversion efficiency was only 3.7%, which is far from those for practical application. Some inappropriate material parameters, such as emitter thickness and doping concentration, may cause the low conversion efficiency. Thus, it is necessary to have a primary understanding of the effects of these parameters to design and fabricate optimal β-$FeSi_2$/c-Si heterojunction solar cells. Numerical simulations of solar cells are particularly useful to accomplish such a task. To the best of our knowledge, published research results about β-$FeSi_2$/c-Si heterojunction solar cells do not deal with this problem. Therefore, a numerical analysis on performance of β-$FeSi_2$/c-Si heterojunction solar cells is carried out in this paper.

In the present work, we concentrate on the effects of β-$FeSi_2$ parameters in the emitter region, which is crucial to cell performance. The effects of layer thicknesses, doping concentrations and recombination parameters of β-$FeSi_2$ have been discussed. The corresponding optimization has been provided for the structure of β-$FeSi_2$/c-Si heterojunction solar cell.

2. Methodologies

Fig. 1 illustrates a schematic structure of β-$FeSi_2$/c-Si heterojunction solar cell in this study.

The simulations of β-$FeSi_2$/c-Si heterojunction solar cells have been performed by PC1D computer program [17], which solves fully coupled nonlinear equations for quasi-one-dimensional transport of electrons and holes in crystalline semiconductor device. The program allows the user to specify all necessary parameters that determine device performance, and it is valid for all levels of injection and fitted well with reported experimental results. The simulated illumination is air mass 1.5, 100 mW/cm^2, and its effective wave band is in the range 380 – 1400 nm. In this work, light reflection of the front and back contacts was set to be 0.1 and 0, respectively. Light absorption coefficients of β-$FeSi_2$ and c-Si are shown in Fig. 2. The absorption coefficient of β-$FeSi_2$ was

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measured by our team. Our measured result is accordant with that in the literature [18,19]. The absorption coefficient of c-Si is obtained from the PC1D program, which has standard data for c-Si absorption coefficient.

In this work, material parameters employed as inputs are selected based on reported literature data [20–24]. The basic semiconductor properties of the β-$FeSi_2$ and c-Si layers for the simulations are shown in Table 1. Front and back contacts are assumed as flat-band ones to neglect the influence of contact potential. Although the interface states have important impact on cell performance, for simplicity they are not taken into account in this simulation.

With carrier concentration varying, the mobility value will be influenced. In order to simulate the performance effects of different carrier concentrations of β-$FeSi_2$, we use the reported

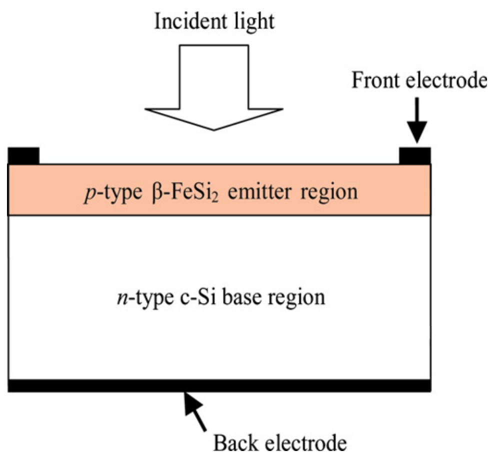

Fig. 1. Schematic structure of β-$FeSi_2$/c-Si hererojunction solar cell in the simulations.

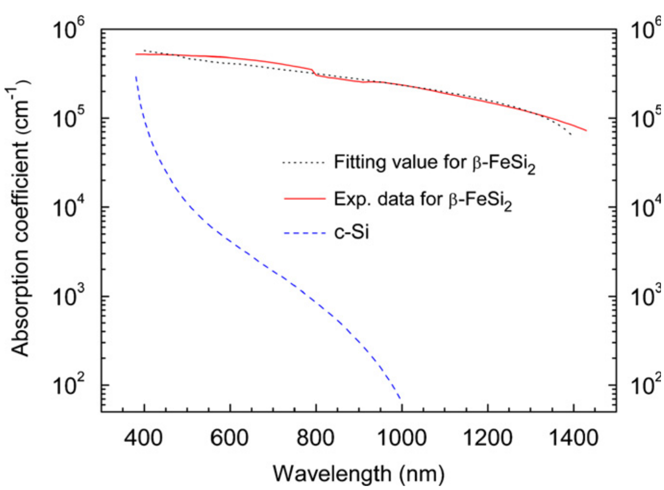

Fig. 2. Light absorption coefficients of β-$FeSi_2$ and c-Si.

Table 1
Basic parameters of β-$FeSi_2$ and c-Si layers at 300 K for the simulations.

Parameter and units	β-$FeSi_2$	c-Si
Thickness (nm)	100 – 500	3×10^5
Acceptor/donor concentration (cm^{-3})	1×10^{16}–3×10^{18}	1×10^{16}
Band gap (eV)	0.87	1.12
Refractive index	5.6	3.58
Intrinsic concentration (cm^{-3})	1.2×10^{12}	1×10^{10}

experimental mobility of β-$FeSi_2$ to fit the Caughey–Thomas empirical formula [25], and the mobility model of c-Si is the default setting that exists in the PC1D software according to the Caughey–Thomas empirical formula. Minority carrier mobilities of p-type β-$FeSi_2$ and n-type c-Si are calculated by the Caughey–Thomas empirical formula:

$$\mu_{\langle e,h\rangle}(N)=\mu_{\min,\langle e,h\rangle}+\frac{\mu_{\max,\langle e,h\rangle}-\mu_{\min,\langle e,h\rangle}}{1+(N_{\langle A,D\rangle}/N_{\mathrm{ref},\langle e,h\rangle})^{\phi_{\langle e,h\rangle}}} \quad (1)$$

In Eq. (1), carrier mobility $\mu_{\langle e,h\rangle}$ is taken as a function of semiconductor doping concentration $N_{\langle A,D\rangle}$ at 300 K; $\mu_{\max}$ and $\mu_{\min}$ are the saturated values of mobilities reached for very low and high doping concentrations, respectively. N_{ref} and ϕ are related fitting parameters. The detailed data are shown in Table 2. Fig. 3 shows the electron mobility of β-$FeSi_2$ and hole mobility of c-Si at 300 K. The mobility of experimental data represented in Fig. 3 by solid triangle is taken from literature [14,26,27] and based on a convenient assumption of equal minority and majority carrier mobilities due to the shortage of minority mobility for β-$FeSi_2$ from the available literature. The calculated results are in good agreement with the experimental data.

The main carrier recombination mechanisms that affect performances of β-$FeSi_2$/c-Si heterojunction solar cells are the radiative, Auger, bulk Shockley–Read–Hall (SRH) and surface recombination. The formulae and related parameters for simulating recombination rates in PC1D for β-$FeSi_2$ are shown in Table 3. The radiative coefficient (B) is calculated [28] without considering photon recycling effect as follows:

$$B=\frac{4\pi n^2}{n_i{}^2}\int_{E_g}^{\infty}\alpha(E)\frac{2E^2}{h^3c^2}\exp\left(\frac{-E}{kT}\right)dE \quad (2)$$

where n is the refractive index, n_i the intrinsic concentration, E_g the band gap, h the Planck constant, c the speed of light in

Table 2
Parameters used in the Caughey–Thomas model for calculating the electron and hole mobilities at 300 K for β-$FeSi_2$ and c-Si.

Materials	Carriers	$\mu_{\max}$ (cm^2/Vs)	$\mu_{\min}$ (cm^2/Vs)	N_{ref} ($\times10^{17}$ cm^3)	ϕ
β-$FeSi_2$	Electron	515	2	0.8	0.93
	Hole	256	0.5	1.2	0.82
c-Si	Electron	1417	60	0.964	0.664
	Hole	470	155	1.0	0.9

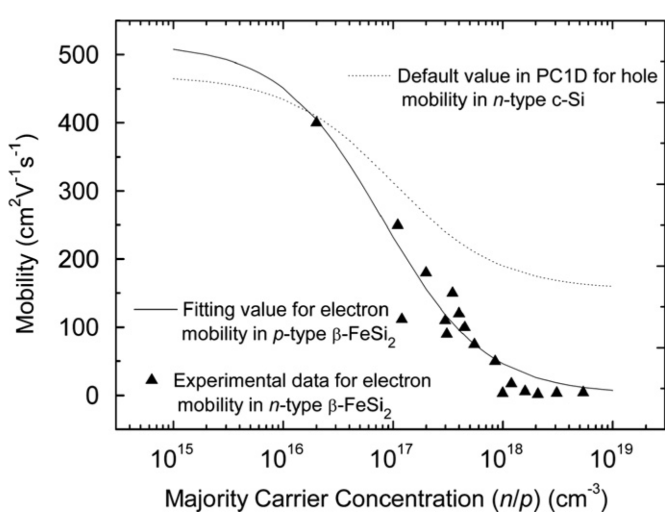

Fig. 3. Electron mobility of β-$FeSi_2$ and hole mobility of c-Si versus doping concentration at 300 K.