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Evaluation of photovoltaic properties of nanocrystalline-$FeSi_2$/Si heterojunctions

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ABSTRACT

In this paper, an application of nanocrystalline iron disilicide (NC-$FeSi_2$) combined with nanocrystalline-Si (NC-Si) in a heterostructured solar cell is introduced and numerically evaluated in detail. The proposed cell structure is studied based on an experimental investigation of photovoltaic properties of NC-$FeSi_2$/crystalline-Si heterojunctions, composed of unintentionally-doped NC-$FeSi_2$ thin film grown on Si substrate. Photoresponse measurement of NC-$FeSi_2$/crystalline-Si heterojunction confirmed ability of NC-$FeSi_2$ to absorb NIR light and to generate photocarriers. However, collection of these carriers was not so efficient and a radical improvement in design of the device is required. Therefore, a modified device structure, comprising of NC-$FeSi_2$ layer sandwiched between two heavily-doped *p*- and *n*-type NC-Si, is suggested and numerically evaluated. Simulation results showed that the proposed structure would exhibit a relatively high conversion efficiency of 25%, due to an improvement in collection efficiency of photogenerated carriers in the NC-$FeSi_2$ and NC-Si layers. To attain such efficiency, defect densities in NC-$FeSi_2$ and NC-Si layers should be kept less than 10^{14} and 10^{16} cm^{-3} eV^{-1}, respectively. Remarkable optical and electrical properties of NC-$FeSi_2$, employed in the proposed structure, facilitate improving device quantum efficiency spectrum providing significant spectrum extension into the near-infrared region beyond Si bandgap.

1. Introduction

The infrared (NIR) spectrum, which includes light wavelengths from 700 to 2500 nm, represents approximately 49% of the solar spectrum (ASTM E891 Solar Spectrum). According to the Shockley-Queisser limit, this may be represented by absorption losses in Si solar cells due to degradation of Si absorption coefficient for the NIR wavelengths [1]. Therefore, in order to increase conversion efficiency of Si photovoltaic cells, extension of the spectral response beyond Si bandgap is indispensable. This could be achieved by introducing additional materials to the cell structure to act as NIR absorption layer. The introduced materials should possess a good NIR response and matched to Si bandgap.

Nanocrystalline iron disilicide (NC-$FeSi_2$), which is a novel semiconducting material comprising $FeSi_2$ nanocrystals with crystal sizes ranging from 3 to 5 nm, has several advantages that serve to resolve the above-mentioned issue: (i) direct and indirect bandgaps of 0.85 eV and 0.74 eV, respectively (corresponding to NIR wavelengths up to 1675 nm), (ii) large absorption coefficient that exceeds 10^5 cm^{-1}, which is ~200-times greater than that of crystalline-Si (c-Si), (iii) its compositional elements (Fe and Si) are from the most abundant elements in the earth's crust, (iv) it is a nontoxic and ecofriendly material, (v) compatible with the current Si technology, and (vi) can be grown on any solid surface at room temperature [2]. These merits adapt to introduce NC-$FeSi_2$ and its crystalline counterpart (β-$FeSi_2$) to be promising candidates for photovoltaic and optoelectronic applications [2–7].

There have been recent numerical simulation reports on $FeSi_2$-based solar cells proposed various device structures, including crystalline-Si (c-Si) combined with the crystalline phase of $FeSi_2$ (β-$FeSi_2$) heterostructure [8–10]. This is to confirm that the orthorhombic β-phase is a promising candidate material for solar cell application. However, from the experimental point of view,

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c-Si is essentially required to grow good quality crystalline β-$FeSi_2$ thin films. Additionally, using c-Si wafers as substrates in these solar cell structures makes them rather expensive. Another proposed structure is a-Si:H/μc-Si/β-$FeSi_2$ tunnel heterojunction solar cell [9]. In practice, triple tunnel junction structure makes use of a tunnel junction of critical importance due to necessity of precise adjustment in the layer thickness and layer doping. Some reports have theoretically used intrinsic-$FeSi_2$, with low carrier densities, in heterojunction structures [8,9]. This might not be a realistic assumption because intrinsic-$FeSi_2$, with that reported carrier density, has never experimentally been obtained so far.

Two coauthors of this report have experimentally studied earlier an infrared photodiode structure consisting of NC-$FeSi_2$ thin film epitaxially grown on c-Si substrate, to exploit the superior light absorption of NC-$FeSi_2$ in the NIR regime [4]. Although the structure evidently proved possibility of adopting NC-$FeSi_2$ in photovoltaic cells, the reported conversion efficiency was relatively low. In the current report, we study reasons of degrading device photovoltaic properties and present alternative solution to improve them. We propose, and numerically evaluate, a modified cell structure excluding c-Si and comprising thin-layers of NC-Si, instead.

NC-Si has been reported to have favorable properties, over those of the traditional hydrogenated amorphous silicon (a-Si:H) used in solar cell applications. These properties include: lower defect density, higher carrier mobility, higher stability due to lower H content, and higher doping efficiency [11–15]. While its mobility is lower than that of polycrystalline-Si, it is preferable due to its easier fabrication and lower growth temperature. NC-Si can be grown on foreign substrates including glass and indium-tenoxide (ITO) substrates. Furthermore, it can be prepared using conventional deposition methods including plasma-enhanced chemical vapor deposition (PECVD) and sputtering [14]. Therefore, this makes NC-Si a promising novel material to be widely used in thin film solar cells.

In our proposed cell structure, NC-Si is used as a window material and visible light absorber in the device. Due to limitation of NC-Si photoresponse in the IR spectrum and its reduced absorption coefficient (less than 1 cm^{-1} for energies lower than 1 eV), NC-$FeSi_2$ is used to absorb NIR light and therefore extends and improves device photoresponse. The device top layer is thin (100 nm) heavily-doped *p*-type NC-Si, while the bottom layer (100 nm) is heavily doped *n*-type NC-Si layer. The main idea is to use these layers to induce a high drift field within the NC-$FeSi_2$ layer, using the Fermi level difference between n^+- and p^+-NC-Si layers. Our simulation results confirmed efficient NIR light absorption and electron-hole pairs (EHPs) generation by the NC-$FeSi_2$ layer.

2. Methodologies

In order to provide a precise study of the device performance, most of material electrical and optical parameters used in device modeling and simulation are realistic, based on experimental measurements [2,4]. Table 1 summarizes electrical parameters of different layers in the device.

Electron affinity of NC-$FeSi_2$ was estimated from experimental measurement of ionization potential of NC-$FeSi_2$ film with a thickness of 350 nm [6]. Carrier density, mobility, and electrical resistivity of NC-$FeSi_2$ were measured as a function of temperature by the Van der Pauw and Hall effect measurements [2]. Optical absorption coefficients of NC-Si and NC-$FeSi_2$ were set according to measured and reported values [15,16]. Furthermore, NC-$FeSi_2$/c-Si *pn* heterojunction device, with an area of 1 cm^2, was fabricated using a facing-targets direct-current sputtering (FTDCS) method. Detailed experimental procedure was explained in a previous report [4]. Here we introduce some physical, electrical, and optical properties of the NC-$FeSi_2$ material and investigate photoresponse of the fabricated device. The photoresponse properties were measured using a Xe lamp (Ushio, UXL-300D) and a monochromator (Oriel 77250) with a focal length of 125 mm and a line density of 600 l/mm. The light intensity was calibrated using commercial photodiodes (Hamamatsu G8372–1 and EOS G030H).

Heavily-doped *n*-type NC-Si/*n*-type NC-$FeSi_2$/*p*-type NC-Si heterojunction solar cell device is proposed as a modified structure to replace c-Si in NC-$FeSi_2$/c-Si device. Devices are simulated using an updated version of Analysis of Microelectronic and Photonic Structures (wx-AMPS) simulation tool [17–19]. The software is generic and versatile one-dimensional semiconductor device simulator that predicts characteristics of electronic and photonic devices using numerical solutions of Poisson's equation, continuity equations, and carrier transport equations in conjunction with sufficient ability to simulate several kinds of material defects. Therefore, the device performance as a solar cell is simulated taking into account different non-idealities effects such as: material defects, trap-assisted tunneling, work functions of front and back contacts, light trapping, and internal reflections at layer interfaces. The latter effect is modeled using dielectric constants and wavelength-dependent absorption coefficients, in order to calculate refractive indices as a function of incident light source frequency. Effect of material defects, either that of NC-$FeSi_2$ layer or Si layers, are numerically simulated starting with Poisson's equation:

$$\frac{d}{dx}\left(\varepsilon(x)\frac{d\Psi}{dx}\right) = q\left[p(x) - n(x) + N_D^+ - N_A^- + p_t(x) - n_t(x)\right] \quad (1)$$

where, ε is the dielectric permittivity of semiconductor as a function of distance x, Ψ is the electrostatic potential, q is the electron charge, p, n are the concentrations of free holes and electrons, N_D^+, N_A^- are the concentrations of ionized donors and acceptors, p_t is

Table 1
Electrical parameters used for device modeling.

Parameter (unit)	Layers		
	p-type NC-Si	*n*-type NC-$FeSi_2$	*n*-type NC-Si
Thickness (nm)	100	350	100
Relative permittivity	11.9	31	11.9
Electron affinity (eV)	4.05	3.86	4.05
Bandgap (eV)	1.12	0.85	1.12
Effective density of states in the conduction band, N_C (cm^{-3})	3.0×10^{19}	2.33×10^{19}	3.0×10^{19}
Effective density of states in the valence band, N_V (cm^{-3})	2.0×10^{19}	2.0×10^{19}	2.0×10^{19}
Electron mobility ($cm^2\ V^{-1}\ s^{-1}$)	40	30	40
Hole mobility ($cm^2\ V^{-1}\ s^{-1}$)	4	1	4
Acceptor concentration, N_A (cm^{-3})	9×10^{18}	1×10^{18}	0
Donor concentration, N_D (cm^{-3})	0	0	9×10^{18}