

# **Modeling the effects of defect parameters on the performance of a p-BaSi<sub>2</sub>/n-Si heterojunction solar cell**

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## Abstract

Barium disilicide ( $\text{BaSi}_2$ ) in thin-film solar cell applications has drawn considerable interest owing to its promising optical and electrical properties. We have achieved an efficiency of 9.9% in p- $\text{BaSi}_2$ /n-Si heterojunction solar cells, which is the highest performance reported among semiconducting silicide devices; however, this value remains much lower than the theoretical limit as defined by the material's band gap. In this paper, we performed numerical simulations based on Silvaco ATLAS to investigate the effects of defect parameters on the performance of heterojunction solar cells. The defects were modeled by introducing two tail bands around the edge of the conduction and valence bands, and an acceptor-like Gaussian distributed localized energy level within the band gap of  $\text{BaSi}_2$ . The influence of the band tail density of states and the parameters of the localized energy levels on the short-circuit current density, open-circuit voltage, fill factor, and efficiency were evaluated. These results enabled us to reproduce the measured  $J$ - $V$  characteristics by simulation.

## Graphical abstract

We propose a defect model of p-BaSi<sub>2</sub> films to reproduce experimentally obtained current-voltage characteristics of p-BaSi<sub>2</sub>/n-Si heterojunction solar cell under AM1.5 illumination. Two band tails and one acceptor-like localized energy level reproduces the experimental result.

## 1. Introduction

Thin-film solar cell materials such as CdTe, CIGS, and organic-inorganic perovskites, have drawn interest for achieving high energy conversion efficiencies  $\eta$  at low-cost [1-4]. However, many of these materials contain rare and/or toxic elements. Hence, there is a need to explore thin-film solar cell materials that are environmentally friendly. Si thin-film solar cells have also been studied; however, it is difficult to achieve  $\eta$  higher than 20% [5-10]. Among many candidate materials, we have focused on semiconducting barium disilicide BaSi<sub>2</sub>, owing to its safe, stable, and abundant constituent elements [11]. BaSi<sub>2</sub> films can be grown by general techniques such as magnetron sputtering, vacuum evaporation, and molecular beam epitaxy [12-15]. BaSi<sub>2</sub> has a suitable band gap  $E_g$  of 1.3 eV [16,17], which matches the solar spectrum, and a high optical absorption coefficient  $\alpha$  of  $3 \times 10^4 \text{ cm}^{-1}$  at 1.5 eV [17,18], which is nearly 40 times as great as that of crystalline silicon. This means that short-wavelength photons are absorbed in the region close to defective surfaces. Therefore, surface passivation is very important to improve  $\eta$  [19]. Moreover, a long minority-carrier lifetime  $\tau$  of approximately 10  $\mu\text{s}$  [20,21] results in a minority-carrier diffusion length  $L$  of approximately 10  $\mu\text{m}$  [22], which is much larger than the grain size of BaSi<sub>2</sub> because of inactive grain boundaries [23]. One unique feature of BaSi<sub>2</sub> is that large values of  $\tau$  and  $L$  can be achieved simultaneously, indicating the great potential of BaSi<sub>2</sub> as a light absorbing layer for thin-film solar cell applications [24]. Several BaSi<sub>2</sub>-based solar cells have been proposed, including BaSi<sub>2</sub> nanowires, back-contacted BaSi<sub>2</sub>, and perovskite/BaSi<sub>2</sub> dual-junction solar cells [25-27]. The carrier conductivity type and concentration can be effectively controlled by impurity doping. In particular, the electron and hole concentrations can be controlled over a wide range between  $10^{16}$  and  $10^{20} \text{ cm}^{-3}$  by Sb and B doping, respectively [5,28,29]. Such high electron and hole concentrations ensure that the material can operate as both electron and hole transport layers in a homojunction solar cell. Numerical simulation and optimization of Si/BaSi<sub>2</sub> heterojunction and BaSi<sub>2</sub> homojunction solar cells have also been reported [30].

Recently, the operation of a BaSi<sub>2</sub> homojunction solar cell has been reported for the first time, showing that the photogenerated carriers in the BaSi<sub>2</sub> layer can be separated by the built-in electric field in a homojunction diode [31,32].

The value of  $\eta$  in p-BaSi<sub>2</sub>/n-Si heterojunction solar cells has approached 10% without any special passivation treatment formed on both Si(111) and Si(001) substrates [33-35]. This value is the highest reported for solar cells fabricated with semiconducting silicides; however,  $\eta$  remains lower than the theoretical limit as defined by its band gap [36]. Deep level transient spectroscopy revealed that undoped n-BaSi<sub>2</sub> films contain a hole trap level with a density of  $1 \times 10^{13} \text{ cm}^{-3}$  at 0.27 eV from the valence band maximum (VBM) [37]. Electron paramagnetic resonance was also found to be an effective means to detect defects in BaSi<sub>2</sub> which carry a charge and have a spin [38]. However, there is almost the lack of information on defects in B-doped p-BaSi<sub>2</sub>. In this work, we performed numerical simulation with the use of Silvaco ATLAS software to model the aforementioned solar cell and clarify the effects of different defect characteristics present in BaSi<sub>2</sub> on the p-BaSi<sub>2</sub>/n-Si heterojunction solar cell performance.

## 2. Model

Silvaco ATLAS software, a physically-based two- and three-dimensional device simulator, treats solar cell performance according to Poisson's equation, the continuity equations of electrons and holes, and transport equations through a defined grid, helping us to understand and depict the physical processes of specified semiconductor structures associated with device operation and make reliable predictions about device behavior [39-43].

The structure and corresponding mesh of the p-BaSi<sub>2</sub>/n-Si heterojunction solar cell is shown in Fig. 1(a). A non-uniform mesh, where the grid is finer around the interface, was defined to obtain good accuracy with a reasonable calculation time. Notably, the BaSi<sub>2</sub> film acts as an emitter of the p-n junction and a light absorbing layer. Figure 1(b) shows schematic

band diagrams of the heterojunction in thermodynamic equilibrium. The conduction-band offset  $\Delta E_C$  and valence-band offset  $\Delta E_V$ , owing to the difference in the electron affinity of BaSi<sub>2</sub> [44] and Si, promote separation of photogenerated carriers in p-BaSi<sub>2</sub> and those in n-Si to ensure good carrier collection.

The accuracy of the material parameters defined in the solar cell model, such as  $E_g$ , electron and hole concentrations ( $n$  and  $p$ ) and carrier mobility ( $\mu_e$  and  $\mu_h$ ) [45], permittivity, affinity, carrier lifetime ( $\tau_e$  and  $\tau_h$ ), and the effective density of states in the conduction and valence bands ( $N_C$  and  $N_V$ ) [46], determine the accuracy of the simulation results. Shockley–Read–Hall (SRH) recombination, which is the main recombination mechanism in BaSi<sub>2</sub> [21], is associated with the Fermi–Dirac statistics and was also considered. We used the experimentally determined carrier mobility [45] and carrier lifetime of BaSi<sub>2</sub> [20,47]. The input parameters for the simulation are given in Table 1 [11]. One of the most important sets of parameters for advanced solar cell modeling is the optical properties containing the refractive index  $n'$  and extinction coefficient  $\kappa$  versus wavelength  $\lambda$ , which decide the transmission and attenuation of light passing through the semiconductor, respectively. The  $n'$  and  $\kappa$  values of BaSi<sub>2</sub> were extracted from experimental results [17,27], where  $\kappa$  was calculated from the relationship  $\alpha = 4\pi\kappa/\lambda$ . Figure 2 shows the absorption coefficient of BaSi<sub>2</sub> and other solar cell materials [27,48-50]. The absorption spectrum of BaSi<sub>2</sub> is similar to that of other thin-film solar cell materials, such as CdTe, CIGS, and CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> in the ultraviolet and visible regions. Notably,  $\alpha$  of BaSi<sub>2</sub> is higher than those of CdTe and CH<sub>3</sub>NH<sub>3</sub>PbI<sub>3</sub> in the near-infrared region. This comparison demonstrates the excellent optical properties of BaSi<sub>2</sub>.

The simulated current density versus voltage ( $J$ - $V$ ) characteristics under AM1.5 illumination for an idealized p-BaSi<sub>2</sub>/n-Si heterojunction solar cell are compared with measurements of a real device in Fig. 3(a). The simulated short-circuit current density ( $J_{SC}$ ) of 39.0 mA/cm<sup>2</sup>, open-circuit voltage ( $V_{OC}$ ) of 0.63 V and  $\eta$  of 15.7% were greater than those of a measured device, which had  $J_{SC}$ ,  $V_{OC}$ , and  $\eta$  being 35.8 mA/cm<sup>2</sup>, 0.47 V, and 9.9%,

respectively [34]. The major difference between these devices is that the simulated device is assumed to be free of defects. The simulation results should match those of the real device; otherwise, the results are not useful for designing and improving real devices. Therefore, to reproduce the measured  $J$ - $V$  characteristics, we introduced defects into the simulated p-BaSi<sub>2</sub> film. In the p-BaSi<sub>2</sub> film, we assumed three components for the density of states (DOS): two band tails exponentially decayed from the conduction band minimum (CBM) and the VBM, one acceptor-like localized energy level characterized by a Gaussian distribution, which created a continuous distribution of trapping centers in the band gap of p-BaSi<sub>2</sub> [51]. The total density of states within the band gap  $g(E)$  is given by [39]:

$$g(E) = G_{TA} \exp\left(\frac{E_V - E}{E_U}\right) + G_{TD} \exp\left(\frac{E - E_C}{E_U}\right) + G_{GA} \exp\left[-\frac{1}{2}\left(\frac{E_{GA} - E}{W_{GA}}\right)^2\right], \quad (1)$$

where  $E_C$  ( $E_V$ ) is the CBM (VBM),  $G_{TA}$  ( $G_{TD}$ ) is the effective density of acceptor (donor)-like tail states,  $E_U$  is the Urbach tail energy [52],  $G_{GA}$  is the effective density of acceptor-like states in a Gaussian distribution,  $E_{GA}$  is the peak energy of the Gaussian distribution of acceptor-like states, and  $W_{GA}$  is the standard deviation of the Gaussian distribution of acceptor-like states. The energies  $E_U$  and  $W_{GA}$  express to what extent those defective states distribute in the energy range. The capture cross-sections for majority carrier (hole) and minority carrier (electron) are set to be  $1 \times 10^{-14}$  and  $1 \times 10^{-16}$  cm<sup>2</sup>, respectively for all states [40]. A schematic representation of such states is shown in Fig. 3(b) with the parameters of the band tails and localized energy level summarized in Table 2. Regarding the Urbach tail energy we fitted the measured absorption spectrum of p-type BaSi<sub>2</sub> films using the empirical rule expressed by [52],

$$\alpha(\hbar\omega) = \alpha_0 \exp\left(\frac{\hbar\omega - E_g}{E_U}\right), \quad (2)$$

where  $\alpha_0$  is constant and  $\hbar\omega$  is the photon energy.  $E_U$  is an inverse logarithmic slope of the Urbach tail, and was found to be approximately 0.10 eV. That's why we set  $E_U$  at 0.10 eV in Table 2. Please note that the series resistance  $R_S$  and the shunt resistance  $R_{SH}$  are not the input

parameters in the simulation even though they can be obtained experimentally by the inverse of the slope of the measured  $J$ - $V$  characteristics at around an open-circuit voltage and 0 V, respectively. They were determined by changing the parameters in Eq. (1) so that the simulation result reproduced the measured  $J$ - $V$  characteristics. We also neglected the contact resistance at the ITO/p-BaSi<sub>2</sub> and Al/n-Si interfaces. This is because they were too small to explain the measured  $R_s$ . Regarding  $R_{SH}$ , ideally, it should be infinitely high. The presence of  $R_{SH}$  means the presence of leakage current. This is caused by recombination of photogenerated carriers via defect levels. They are also determined by parameters in Eq. (1).

### 3. Results and discussion

From the introduced defect model, we first investigated the effects of the defect parameters  $G_{TA}(G_{TD})$ ,  $E_U$ ,  $G_{GA}$ ,  $E_{GA}$ , and  $W_{GA}$  on solar cell performance. We considered the effects of the above-mentioned parameters individually, while maintaining other parameters constant, as defined in Table 2. The localized defect level located at 0.37 eV above the valence band edge can be linked to acceptor-like impurities, such as dangling bonds in the Si tetrahedra of the BaSi<sub>2</sub> lattice, neutral non-ionized boron or oxygen atoms [51,53,54].

#### 3.1 Urbach tail energy

Although the Urbach tail energy  $E_U$  was obtained to be 0.10 eV, we varied it symmetrically from 0.02 to 0.20 eV for the CBM and VBM to see its influence on the  $J$ - $V$  characteristics. The  $J$ - $V$  curves of the simulated solar cell versus  $E_U$  are shown in Fig. 4. The  $V_{OC}$  does not change with  $E_U$ , meaning that  $E_U$  does not have a major effect on the solar cell performance.

#### 3.2 Density of states of band tails

We next discuss the effect of band tail density of states  $G_{TA}(G_{TD})$  on the solar cell



performance. Here, the conduction and valence band tails are considered to be symmetric, that is  $G_{TA}(E) = G_{TD}(E_C - E)$ , and was varied from  $1 \times 10^{13}$  to  $1 \times 10^{23} \text{ cm}^{-3} \text{ eV}^{-1}$ . At the same time, the DOS of the acceptor-like localized energy level was maintained at  $G_{GA} = 1 \times 10^{15} \text{ cm}^{-3} \text{ eV}^{-1}$  and hence has a negligible effect on the solar cell performance. The simulated  $J$ - $V$  curves are shown in Fig. 5(a). Figure 5(b) shows the  $J_{SC}$ ,  $V_{OC}$ ,  $FF$ , and  $\eta$  as a function of  $G_{TA}$  ( $G_{TD}$ ), as extracted from the  $J$ - $V$  curves. These four parameters remained unchanged with  $G_{TA}$  ( $G_{TD}$ ) up to  $1 \times 10^{20} \text{ cm}^{-3} \text{ eV}^{-1}$ . When  $G_{TA}$  ( $G_{TD}$ )  $> 10^{20} \text{ cm}^{-3} \text{ eV}^{-1}$ , the solar cell performance started to degrade. The degradation of the  $J_{SC}$  can be explained by the fact that the photogenerated carriers are captured by the more densely distributed defects. Simultaneously, the values of  $FF$  and  $\eta$  markedly decreased and the shape of the  $J$ - $V$  curves takes on an  $S$ -shape, indicating the presence of a barrier at the p-BaSi<sub>2</sub>/n-Si interface. This result demonstrates that defects may act as dopants, which modify the doping profile and reduce the depletion region around the junction. The main difference between the ideal and measured p-BaSi<sub>2</sub>/n-Si heterojunction solar cells is the magnitude of  $V_{OC}$ , in that the simulated  $J$ - $V$  curves do not match those measured for the device by changing only  $E_U$  and  $G_{TA}$  ( $G_{TD}$ ).

### 3.3 Standard deviation of the Gaussian distribution of localized energy level

$W_{GA}$  corresponds to the defect dispersion, which shows the energy range where the localized energy levels are located within the band gap. The simulated  $J$ - $V$  curves are shown in Fig. 6(a). Here,  $W_{GA}$  ranged from 0.04 to 0.57 eV and  $G_{GA}$  was maintained at  $1 \times 10^{15} \text{ cm}^{-3} \text{ eV}^{-1}$ . When the value of  $W_{GA}$  increased,  $J_{SC}$  and  $V_{OC}$  remained unchanged. We speculate that this result can be attributed to  $G_{GA}$  and  $E_{GA}$  being set at constant values. However, the values of  $FF$  and  $\eta$  decreased markedly when  $W_{GA}$  was larger than 0.2 eV. Figure 6(b) shows the response of  $FF$  and  $\eta$  to  $W_{GA}$ . The decrease of  $FF$  with increasing  $W_{GA}$  can be explained by the increase of  $R_S$  modeling the resistive losses of materials and the decrease of  $R_{SH}$  representing an increase of the parasitic leakage current that crosses the cell. The increase of

$W_{GA}$  enhances the recombination of photogenerated carriers via defect levels, resulting in a decrease of  $R_{SH}$ . Lock-in thermography used for crystalline Si solar cells may also give us information about leakage currents in BaSi<sub>2</sub> solar cells [55].

### 3.4 Peak energy of localized energy level from valence band

The next defect parameter is  $E_{GA}$ , the peak energy of the acceptor-like localized states within the band gap of BaSi<sub>2</sub>. This parameter was varied from 0.1 to 0.6 eV above the VBM. The obtained  $J$ - $V$  curves are shown in Fig. 7(a). The values of  $J_{SC}$  slightly increased and the degradation can be attributed to a decrease in  $V_{OC}$ . This phenomenon can be explained as follows: when the defect level shifts from 0.1 to 0.6 eV from the VBM, band-to-defect transitions may occur, leading to degradation of the effective band gap in BaSi<sub>2</sub>. Such degradation decreases the  $V_{OC}$ . These results suggest that the peak energy of localized states strongly affects the  $V_{OC}$ . In our case, the main difference between the ideal and measured p-BaSi<sub>2</sub>/n-Si heterojunction solar cell is in the  $V_{OC}$ . Thereby, a value of  $E_{GA} = 0.4$ – $0.5$  eV is needed to reproduce the measured  $J$ - $V$  curve.

### 3.5 Density of states of localized energy level

The last studied defect parameter is the DOS of acceptor-like localized energy level  $G_{GA}$  into the BaSi<sub>2</sub> film, which was varied from  $1 \times 10^{13}$  to  $1 \times 10^{20}$  cm<sup>-3</sup> eV<sup>-1</sup>. The simulated  $J$ - $V$  curves are shown in Fig. 8(a). Figure 8(b) shows the  $J_{SC}$ ,  $V_{OC}$ ,  $FF$ , and  $\eta$  as a function of  $G_{GA}$ , extracted from the  $J$ - $V$  curves. The values of  $J_{SC}$  and  $V_{OC}$  do not change when  $G_{GA}$  is below  $1 \times 10^{18}$  cm<sup>-3</sup> eV<sup>-1</sup>. As  $G_{GA}$  increases above  $1 \times 10^{18}$  cm<sup>-3</sup> eV<sup>-1</sup>, the presence of a localized energy level in the BaSi<sub>2</sub> film degrades the solar cell performance. Apparently, the effect of acceptor-like localized energy states with a Gaussian distribution is very similar to that of tail states. The reduction of  $J_{SC}$  can be reasonably understood by considering that the photogenerated carriers are trapped by the energy level. The degradation of the  $V_{OC}$  can be

explained by a decrease in  $J_{SC}$  and a possible increase of the dark saturated current density  $J_S$  of the heterojunction in the presence of defects in accordance with the relationship:  $V_{OC} = k_B T / q \ln (J_{SC} / J_S)$ . Simultaneously, the presence of a barrier at the p-BaSi<sub>2</sub>/n-Si interface results in a decrease of  $FF$  and  $\eta$ . In general, defect parameters of the localized energy level have a stronger influence on solar cell performance than band tail parameters.

### 3.6 Reproduction of the measured $J$ - $V$ curve

The defect effects of band tails and the localized energy levels in the BaSi<sub>2</sub> film led to comparable values between the simulation and measured results. A comparison of the  $J$ - $V$  curves is shown in Fig. 9(a) with defect parameters values:  $G_{TA}(G_{TD}) = 1.2 \times 10^{18} \text{ cm}^{-3} \text{ eV}^{-1}$ ,  $E_U = 0.10 \text{ eV}$ ,  $G_{GA} = 3.5 \times 10^{17} \text{ cm}^{-3} \text{ eV}^{-1}$ ,  $W_{GA} = 0.06 \text{ eV}$ , and  $E_{GA} = 0.45 \text{ eV}$ , as plotted in Fig. 9(b). A good agreement was obtained between the simulation and measurements. We should note however that there is still a large divergence of curves in the current density range 20 to 33 mA/cm<sup>2</sup>. Since the bending is very sensitive to model and physical processes responsible for the performance of solar cells, such divergence is a sign that either the model is too much simplified and additional parameters or processes should be considered or another set of numerical values should be used for those adjustable parameters. Thus, further studies are mandatory to reach a better fitting. Anyway, we confirmed that the defects are the main origin of the degradation of the p-BaSi<sub>2</sub>/n-Si heterojunction solar cell performance. According to first-principle calculations based on the density-functional theory [51], B atoms occupy not only Si sites but also interstitial sites in BaSi<sub>2</sub>, leading to the formation of deep localized states within the band gap of BaSi<sub>2</sub>. Thereby the value of  $E_{GA} = 0.45 \text{ eV}$  from the VBM is considered reasonable. The defect density of localized states  $N_T$  was calculated from  $G_{GA}$  and  $W_{GA}$  using Eq. (1) to be approximately  $5 \times 10^{16} \text{ cm}^{-3}$ . Recently, supplying atomic H to BaSi<sub>2</sub> films has been found to effectively reduce the defects in undoped BaSi<sub>2</sub> films and markedly enhance the minority-carrier lifetime [56,57]. Thus, further studies on passivating BaSi<sub>2</sub> films

with atomic H might lead to higher  $\eta$  values.

#### 4. Conclusion

In this paper, we used a numerical simulation, based on Silvaco ATLAS software, to model a p-BaSi<sub>2</sub>/n-Si heterojunction solar cell and establish a reliable defect model to reproduce experimentally obtained  $J$ - $V$  curve. Two band tails and one acceptor-like localized energy level were taken into consideration. We analyzed the effect of the Urbach tail energy, density of states of band tails, and density of the localized energy level in the band gap of BaSi<sub>2</sub>. The peak energy and the standard deviation of the Gaussian distribution of the localized energy level had a considerable influence on  $V_{OC}$  and  $FF$ , respectively. Experimental  $J$ - $V$  curves were well reproducible by simulations when the defect parameters were set as follows: a density of tail states  $G_{TA}(G_{TD}) = 1.2 \times 10^{18} \text{ cm}^{-3} \text{ eV}^{-1}$ , a decay energy of the tail states  $E_U = 0.10 \text{ eV}$ , a density of localized states  $G_{GA} = 3.5 \times 10^{17} \text{ cm}^{-3} \text{ eV}^{-1}$ , a standard deviation of Gaussian distribution of the localized states  $W_{GA} = 0.06 \text{ eV}$ , and a peak energy of the localized states  $E_{GA} = 0.45 \text{ eV}$ .

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Table 1 Input parameters for simulation [11].

Material	p-BaSi <sub>2</sub>	n-Si
$d$ [nm]	20	$2 \times 10^5$
$E_g$ [eV]	1.3[16,17]	1.1
$n$ [cm <sup>-3</sup> ]	–	$2 \times 10^{15}$
$p$ [cm <sup>-3</sup> ]	$2 \times 10^{18}$	–
Permittivity	14.0[46,48]	11.7
Affinity [eV]	3.2[44]	4.05
$N_C$ [cm <sup>-3</sup> ]	$2.6 \times 10^{19}$ [46]	$2.8 \times 10^{19}$
$N_V$ [cm <sup>-3</sup> ]	$2.0 \times 10^{19}$ [46]	$1.0 \times 10^{19}$
$\tau_e$ [μs]	8[20]	1.5
$\tau_h$ [μs]	8[47]	1.5
$\mu_e$ [cm <sup>2</sup> /Vs]	500[45]	1000
$\mu_h$ [cm <sup>2</sup> /Vs]	30[45]	500

Table 2 Parameters of the band tails and localized energy level.

	Band tails	Localized energy level
Urbach tail energy [eV]	0.10	–
Density of states [ $\text{cm}^{-3}\text{eV}^{-1}$ ]	$1.0 \times 10^{16}$	$1.0 \times 10^{15}$
Peak energy from the VBM [eV]	–	0.37

Figure captions

Fig. 1. (a) Schematic diagram and defined mesh and (b) band alignment of the p-BaSi<sub>2</sub>/n-Si heterojunction solar cell.

Fig. 2. Absorption coefficient of BaSi<sub>2</sub> and other solar cell materials [27,49,50].

Fig. 3. (a)  $J$ - $V$  curves of simulated ideal and measured p-BaSi<sub>2</sub>/n-Si heterojunction solar cell [34]. (b) Schematic of the band tails and the acceptor-like localized energy levels in BaSi<sub>2</sub> band gap.

Fig. 4. Simulated  $J$ - $V$  curves as a function of Urbach tail energy  $E_U$ .

Fig. 5. (a) Simulated  $J$ - $V$  curves as a function of  $G_{TA}$  ( $G_{TD}$ ).  $G_{GA}$  was set to be  $1 \times 10^{15} \text{ cm}^{-3} \text{ eV}^{-1}\text{s}$ . (b) Solar cell parameters  $\eta$ ,  $FF$ ,  $V_{OC}$ ,  $J_{SC}$  extracted from (a).

Fig. 6. (a) Simulated  $J$ - $V$  curves as a function of  $E_U$ .  $G_{GA}$  was kept at  $1 \times 10^{15} \text{ cm}^{-3} \text{ eV}^{-1}$ . (b) Solar cell parameters  $FF$  and  $\eta$  against  $E_U$ , extracted from (a).

Fig. 7. (a) Simulated  $J$ - $V$  curves as a function of peak energy of localized energy level  $E_{GA}$ . (b) Dependence of  $V_{OC}$  against on  $E_{GA}$ .

Fig. 8. (a) Simulated  $J$ - $V$  curves as a function of density of states of localized energy level  $G_{GA}$ . (b) Solar cell parameters  $\eta$ ,  $FF$ ,  $V_{OC}$ ,  $J_{SC}$  of p-BaSi<sub>2</sub>/n-Si solar cells, extracted from (a).

Fig. 9. (a) Comparison of simulated and measured  $J$ - $V$  characteristics of the p-BaSi<sub>2</sub>/n-Si heterojunction solar cell. (b) Defect model in p-BaSi<sub>2</sub> used for simulation in (a).

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(a)

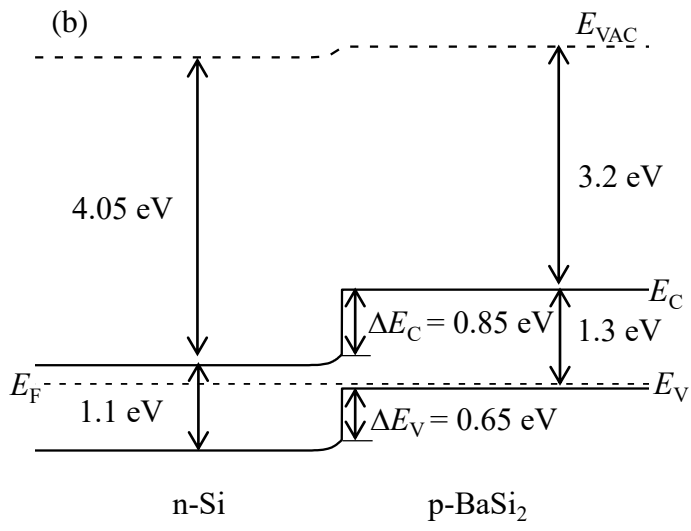
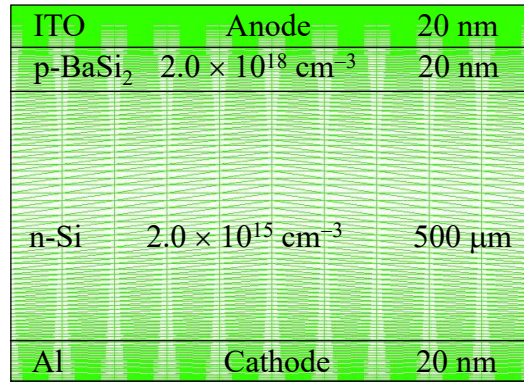


Fig. 1

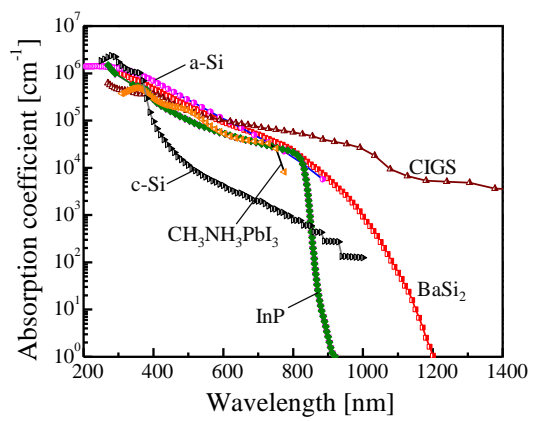


Fig. 2

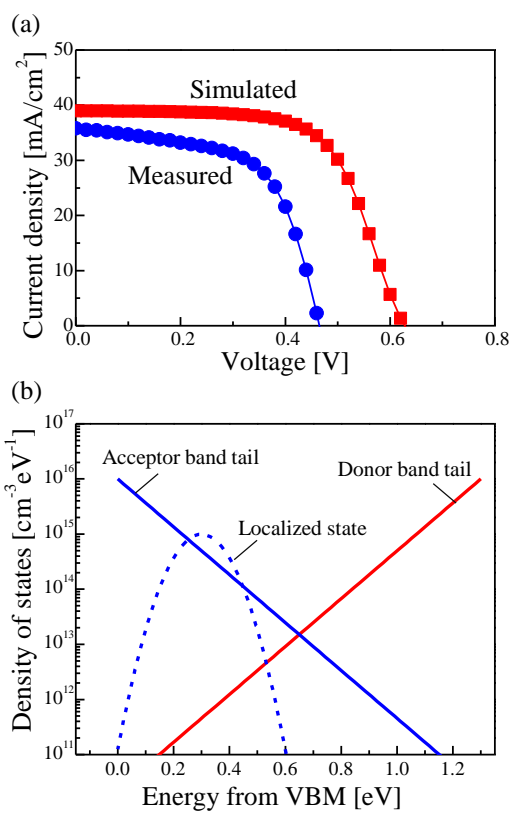


Fig. 3

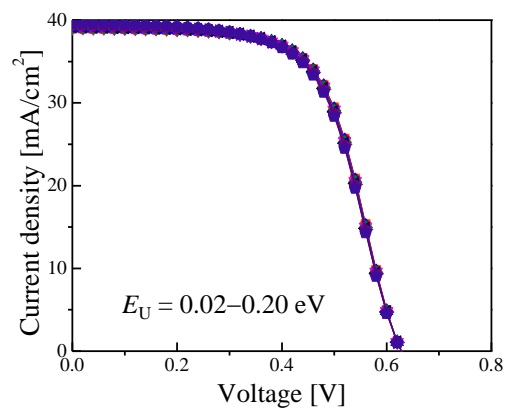


Fig. 4



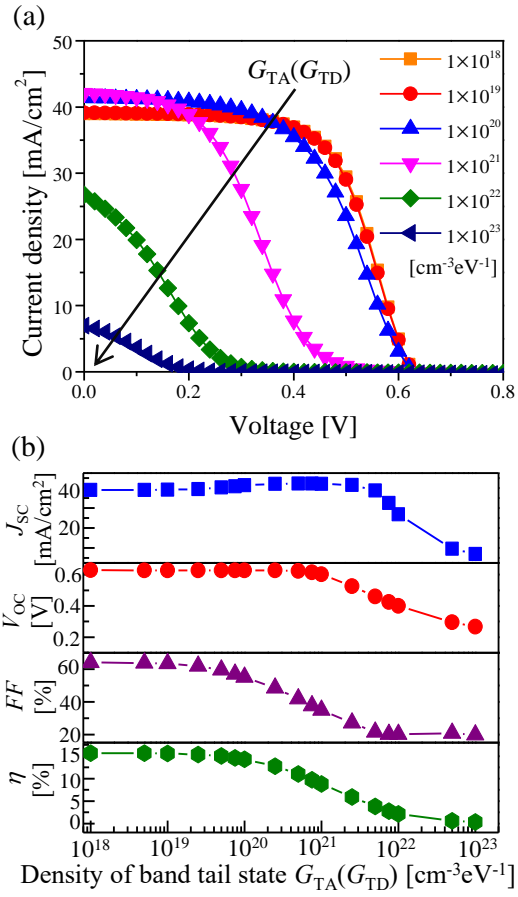


Fig. 5

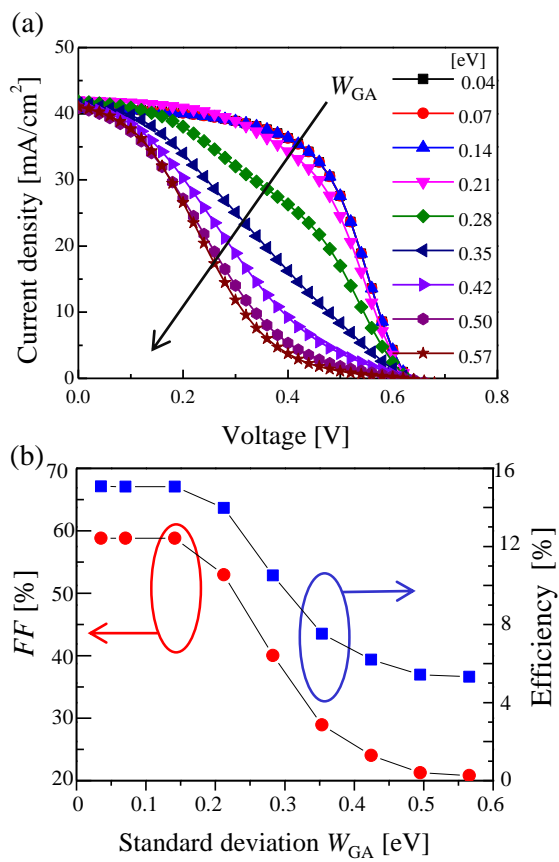


Fig. 6

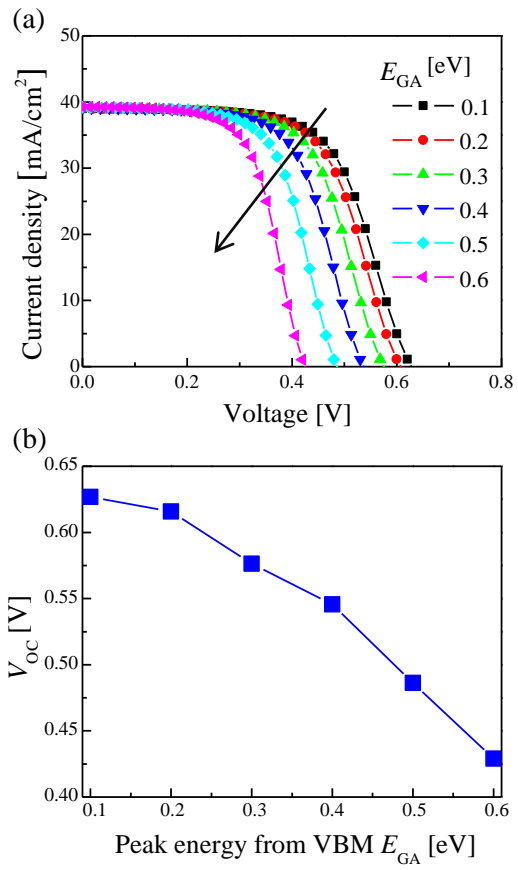


Fig. 7

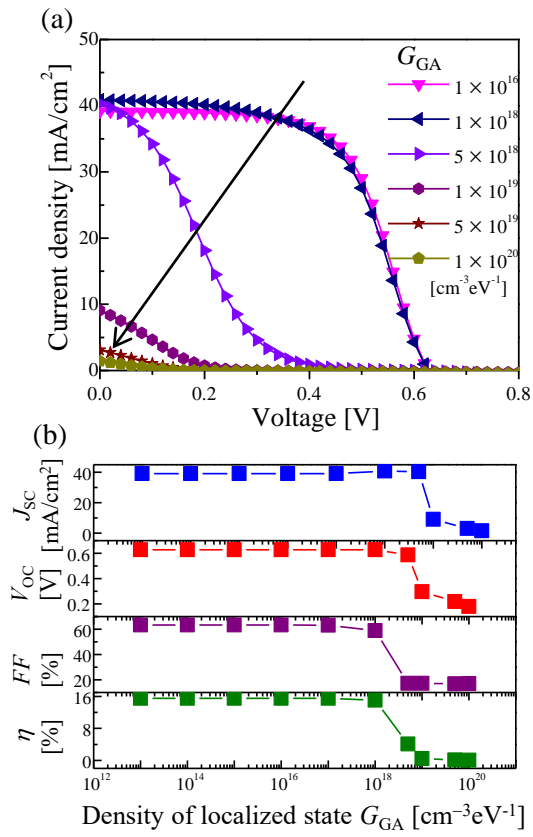


Fig. 8

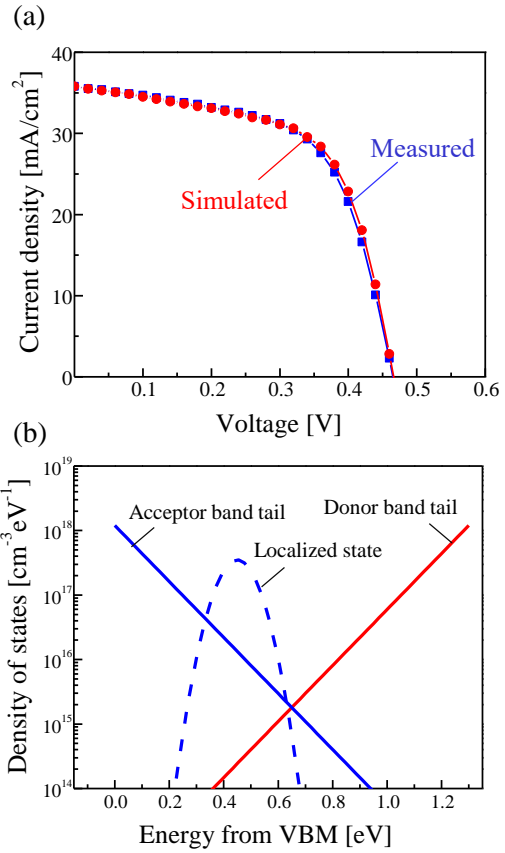


Fig. 9