



Band structure adjustment of solar cells by gradient doping



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ABSTRACT

This paper presents a study of the influence of gradient doping on solar cell performance. The gradient doping of the emitter layer of a a-Si:H(n)/a-Si:H(i)/c-Si(P) solar cell was simulated using the AFORS-Het software simulation package. Band structure adjustment due to gradient doping was studied. The adjustment manifests itself in two separate ways: the gradient quasi-Fermi level splitting (ΔE_F) and the gradient band slope. The relationship between ΔE_F and doping concentrations has been theoretically deduced and simulated using the AFORS-Het software package. The study shows that the ΔE_F caused by gradient doping can improve the spectral response of the cell at long wavelengths and enhance the open circuit voltage. The steeper energy band caused by the higher doping gradient, G , promotes the effective separation of the carriers and reduces their recombination by 2–3 orders of magnitude compared to that of the uniform band. The photovoltaic conversion efficiency of the silicon heterojunction solar cell increases from 13.65% (uniform doping) to 20.86% for the gradient doping cell with the highest G and steepest energy band. This numerical simulation shows that the band structure adjustment caused by gradient doping can achieve higher utilization of solar energy and suppress the recombination of the carriers at the heterojunction interface. The study will guide practical preparation of future solar cells.

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1. Introduction

Fabrication of a high-efficiency solar cell requires the use of a wider range of the solar spectrum and suppression of recombination at the a-Si:H/c-Si interface. By adding a thin intrinsic a-Si:H buffer layer, forming a heterojunction with an intrinsic thin layer (HIT), the interface states and recombination were reduced, resulting in a 23% higher efficiency than that achieved by the Sanyo group. To further enhance the utilization of sunlight and suppress the recombination, energy band engineering has been applied to solar cell design by increasing the photon absorption and the carrier collection capability, e.g., introducing a graded band-gap in the absorbing layer using

polymorphous silicon with different structural characteristics [1], and adjusting the conduction band offset by changing the electron affinity of the solar cell window layer [2,3].

Doping is a very important process used to improve the properties of semiconductors [4–6], and the band structure of solar cells could be adjusted using gradient doping. First, the additional electric field caused by gradient doping can change the electronic potential and adjust the band structure [7]; second, doping can influence the quasi-Fermi level, and in the unbalanced process of photovoltaic conversion, the splitting of the quasi-Fermi level ($\Delta E_F = \epsilon_{fC} - \epsilon_{fV}$) determines the upper limit of the open circuit voltage [8].

The maximum power point for photovoltaic conversion of monochromatic light is related to the chemical potential μ_{eh} (equal to ΔE_F) of the photo-generated electron and hole. The maximum power point for low-energy photon

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appears at a low energy of μ_{eh} [9]. A gradient quasi Fermi level splitting can improve the utilization of the solar energy, especially improving the spectral response intensity at long wavelengths. $\Delta\epsilon_F$ must gradually decrease with the position from the surface to the deeper part of the absorbing layer. Bremner, et al., pointed out in 1999 that the quasi-Fermi level regulation plays a key role in improving the efficiency of solar cells [10]. Solar cells with gradient quasi Fermi levels were proposed to break the traditional efficiency limit by adjusting the solar spectral response. The theoretical efficiency of 63% for a solar cell with a potential well layer of GaAs was far beyond the theoretical efficiency limit (45%) of the multi-stack solar cell [11].

If the $\Delta\epsilon_F$ adjustment can be achieved by doping, the solar cell properties can be enhanced. The purposes of this research are twofold: a) deducing the relationship between $\Delta\epsilon_F$ and doping, and b) exploring the influence of the splitting $\Delta\epsilon_F$ and the energy band adjustment on the suppression of the recombination and enhancement of the solar energy utilization.

2. Theory

Based on the physical model of PN junctions and the carrier transport equations, the relationship between the doping and the Fermi level split was determined. The recombination of carriers via impurity levels is the predominant process in solar cells, and the relationship between the doping concentration and the Fermi level split can be obtained by examining this process. The non-equilibrium carrier concentration with a Fermi distribution can be expressed as follows [5]:

$$n_e = n_i \exp\left(-\frac{\epsilon_i - \epsilon_{FC}}{\kappa T}\right) \quad (1)$$

$$n_h = n_i \exp\left(-\frac{\epsilon_{FV} - \epsilon_i}{\kappa T}\right) \quad (2)$$

where n_e and n_h represent the concentration of electrons and holes, respectively. In an n-type semiconductor, the electron is the majority carrier and the light absorption of the solar cell can be seen as a small injection condition. Considering fully ionized impurities, the photo-generated carrier $n_e \approx n_{e0} \approx n_{imp} \gg \Delta n$, $n_h \approx \Delta p \gg n_{h0}$ (n_{e0} , n_{h0} are the electron and hole concentrations under equilibrium conditions, n_{imp} is the impurity concentration, Δn and Δp represent the nonequilibrium carriers arising from the injected light), and Eqs. (1) and (2) above can be expressed as follows:

$$n_{imp} = n_e = n_i \exp\left(-\frac{\epsilon_i - \epsilon_{FC}}{\kappa T}\right) \quad (3)$$

$$n_h = \Delta p = n_i \exp\left(-\frac{\epsilon_{FV} - \epsilon_i}{\kappa T}\right) \quad (4)$$

Combining the two Eqs. (3) and (4), it can be deduced that

$$n_{imp} = \exp\left(\frac{\epsilon_{FC} - \epsilon_{FV}}{\kappa T}\right) / \Delta p \quad (5)$$

In the fixed-illumination environment, the number of photo-generated holes Δp can be also regarded as a constant. Rewriting Eq. (5)

$$n_{imp} = K \exp\left(\frac{\epsilon_{FC} - \epsilon_{FV}}{\kappa T}\right) \quad (6)$$

It can be deduced that the linear adjusting of the split $\Delta\epsilon_F$ can be created by exponential mode doping of n_{imp} . This offers us the opportunity to adjust $\Delta\epsilon_F$ by doping concentration n_{imp} . The study of the electric field of the gradient-doped solar cells in the literature [7] shows that the exponential doping is superior to the linear doping for improving the electric field of the solar cell when the total doping concentration is fixed. Our calculation shows that linear change of the split $\Delta\epsilon_F$ can be achieved by doping with exponential mode, which can also improve the conversion efficiency of solar cells.

AFORS-HET simulates and analyses the properties of heterojunction solar cells through solving the one-dimensional Poisson equation and the transport equation for electrons and holes with the help of finite differences [12]. The electron/hole currents are driven by the gradient of the corresponding quasi Fermi energy $E_{Fn,p}$, and equivalent to the sum of a diffusion and a drift current with the corresponding mobility $\mu_{n,p}$. The double effect of the exponential doping on the improvement the electric field and the adjustment of the split $\Delta\epsilon_F$ of the solar cell was studied using AFORS-HET simulation.

3. Structure of solar cells and simulation details

In our numerical simulation of the a-Si:H(n)/a-Si:H(i)/c-Si(P) solar cell, we considered three main defect types [12]. We assumed that there are no recombination currents at the ideal c-Si/a-Si:H interface. A solar illumination of AM1.5 (power density 100 mW/cm²) was used as a light source. Other parameters used in the simulations are shown in Table 1 [13,14]. The methods of achieving the exponential doping can be seen in our previous study [15]. Although the more layers the emitter is divided into, the closer the doping is to the exponential mode, further subtle division would bring increased calculation difficulty. Our previous study indicated that with the gradual increase of the division layers from 7 to 10 layers [15], there are no obvious influence on the solar cell performance. In our simulation, the emitter is divided into only 10 layers.

The doping concentration of one divided layer is the same, and obtained by summing the exponential doping data included in that divided layer. While the doping concentration of different divided layer is not the same, an average doping concentration, N_d , was used to compare the different solar cells, and expressed as $N_d = Ct/He$ based on one-dimensional simulation. Ct , He is the total doping content and the thickness of the emitter, respectively. He is the same for all the studied cells in the paper, so that introducing a parameter $G = C_1 - C_2$ to describe the doping gradient is reasonable. C_1 is the doping concentration of the first divided layer in the emitter layer near the solar cell surface, and C_2 is the concentration of the last layer close to a-Si:H passivation layer.

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