A novel α -Si : H solar cell designed by two-dimensional device simulation

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Abstract. The performance of a novel hydrogenated amorphous silicon (α -Si : H) solar cell that utilizes the field effect (field effect solar cell (FESC)) has been investigated theoretically. The analysis has been done for both p - and n -channel FESCs, employing a two-dimensional device simulator which is based on current continuity and Poisson equations. The calculation predicted that both n -channel and p -channel FESCs could offer improved conversion efficiency as compared with the conventional-doped p - i - n solar cell with equal quality i (intrinsic)-layer. The observed improvement can be mainly attributed to the quantum-efficiency increase for high-energy photons. Cell parameters that may affect the energy conversion efficiency of FESCs have also been evaluated with the simulator.

Keywords. Two-dimensional device simulation; field effect; α -Si : H; solar cell.

1. Introduction

Amorphous silicon (α -Si : H) solar cell is a promising candidate for future low-cost solar-power-generation device. Its conversion efficiency is however relatively low as compared with that of the crystalline silicon solar cells. One main reason for this low-conversion efficiency is the large absorption of short-wavelength light at the heavily doped p -type window layer, which even if it is as thin as 20 nm can result in high recombination of photo-generated carriers.

Recently, we have proposed a new type of α -Si : H solar cell which is schematically illustrated in figure 1 (Koinuma *et al* 1996). This field effect solar cell (FESC) utilizes an inversion layer, which is induced by the field effect, instead of impurity-doped p -type window layer. By applying a negative voltage on the front transparent conducting oxide (TCO) layer with respect to the back metal electrode, it is possible to induce a p -type channel at the top of i -layer contacting with the TCO. The generated electricity thus by the conversion of sunlight can be utilized by placing a load between the comb electrode and the back-side metal electrode. The use of a ferroelectric oxide, instead of a dielectric material, is attractive since the effect of the induced p -channel remains even after the bias is removed. Furthermore, the cell can be operated as an n -channel device by replacing the n -type α -Si : H bottom layer with p -type α -Si : H. In addition to the presumed advantage of using an undoped-

p (or $-n$) channel, we have the freedom of using comb electrode with an appropriate work function. This paper describes the performance of FESC structures, based on a two-dimensional device simulation, as well as focuses on the effect of device parameters.

2. Device simulation

Since the FESC involves carrier motion in lateral as well as in vertical directions to the surface, two-dimensional device simulation is carried out by using a device simulator (SILVACO's ATLAS) based on the simultaneous solution of the carrier continuity equation and the Poisson equation. In addition to the device simulation for the p -channel and n -channel FESCs, we have also calculated the performance of a conventional p - i - n cell for comparison. Although the formation of the surface inversion layer can be achieved either by the use of a fixed charge in the insulator (Hezel and Schörner 1981) or by the application of bias to the dielectric or the ferroelectric material, we chose the bias application to the dielectric layer for simplicity in our simulation.

For simulation of such a defective material as α -Si : H, it is important to model a deep level in the energy gap appropriately. We assumed the exponential tail and Gaussian localized distribution (Shaw and Hack 1988). While on ionization, the donor-like trap concentrations acquire a positive charge, the acceptor-like trap concentrations acquire a negative charge. No additional trap is assumed at the insulator/ α -Si : H interface, since our cell can avoid problems

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of the interphase traps by applying a high electric field on TCO (Kuwano *et al* 1981).

The Poisson's equation and hole- and electron-continuity equations used in this simulation are expressed by (1) and (3), respectively.

$$\epsilon \nabla^2 \psi = -q(p - n + N_D - N_A + \int_{E_v}^{E_c} N_{t_D}(E) f(E) dE - \int_{E_v}^{E_c} N_{t_A}(E) f(E) dE), \quad (1)$$

and where,

$$f(E) = \frac{n \sigma_n v_{th} N_t(E) + \sigma_p v_{th} N_t(E) n_{ie} \exp(-E/kT)}{\sigma_n v_{th} N_t(E) \{n + n_{ie} \exp(E/kT)\} + \sigma_p v_{th} N_t(E) \{p + n_{ie} \exp(E/kT)\}} \quad (2)$$

$$\frac{\partial n}{\partial t} = \frac{1}{q} \bar{\nabla} \cdot \bar{J}_n - U, \quad (3a)$$

$$\frac{\partial p}{\partial t} = \frac{1}{q} \bar{\nabla} \cdot \bar{J}_p - U, \quad (3b)$$

and where,

$$U = \int_{E_v}^{E_c} \frac{pn - n_{ie}^2}{\frac{n + n_{ie} \exp(E/kT)}{\sigma_p v_{th} N_t(E)} + \frac{p + n_{ie} \exp(E/kT)}{\sigma_n v_{th} N_t(E)}} dE, \quad (4)$$

$$\bar{J}_n = -q \mu_n n \bar{\nabla} \phi_n, \quad (5a)$$

and

$$\bar{J}_p = q \mu_p p \bar{\nabla} \phi_p. \quad (5b)$$

In (1), ϵ the permittivity of *a*-Si:H, ϕ the electrostatic potential, q the electron charge, n and p are the electron and hole concentrations, N_D and N_A are the ionized donor and acceptor concentrations, $N_{t_D}(E)$ and $N_{t_A}(E)$ are the donor-like and acceptor-like trap concentrations, $f(E)$ the trap occupation function, E_c the conduction edge energy, E_v the valence top energy. In (2), σ_n and σ_p are the capture cross-section for electrons and holes, k the

Boltzmann constant, v_{th} the thermal velocity of carriers, $N_t(E)$ the density of trap centre, T the temperature, and n_{ie} is the intrinsic carrier concentration of *a*-Si:H. In (3) to (5), $\bar{J}_n$ and $\bar{J}_p$ are the electron and hole currents, U the recombination rate, μ_n and μ_p are the electron and hole mobilities, and ϕ_n and ϕ_p are the quasi-Fermi potentials for electrons and holes.

Equation (2) is the accurate Shockley-Read-Hall expression (Hall 1952) to obtain the trap occupation function. Equation (4) is the recombination rate for this material calculated using the Shockley-Read-Hall expression and (5a) and (5b) are the electron and hole currents, respectively.

For the device simulation of this structure, there are many structural parameters that may affect the energy conversion efficiency. Among them, the intrinsic (*i*) layer thickness and the distance between the comb-electrodes being the key parameters, they were varied from typical values of 0.5 μm and 30 μm , respectively. The width of the comb front contact was fixed at 1 μm . The mobility gap of *a*-Si:H was assumed to be 1.7 eV and the absorption coefficients were the same as the values reported by Piller (1985), respectively. Other properties were taken from Chatterjee (1994) and Koinuma *et al* (1996). Device parameters used in the calculation are summarized in table 1.

3. Results and discussion

Figure 2 shows the energy band diagrams calculated for the FESC and conventional cell along the vertical centre of the cells (see figure 1). In the conventional *p-i-n* cell, a negative electric field is induced in the *p*-type window layer, driving electrons from TCO to *p*-type *a*-Si:H layer. Hence, most of the electrons photo-generated in the *p*-type layer are trapped at the TCO/*a*-Si:H interface, rather than being driven towards the *i*-layer and consequently cannot generate a photocurrent. In contrast, there is no negative electric field at the vertical centre for the field effect cell, which results in high collection efficiency for carriers. An increase up to 35% in the short circuit current (I_{SC}) can be accounted in terms of photons absorbed in the 200 Å-thick impurity-doped window layer. This can be a significant effect, especially for photons with high energies, since most of them are absorbed near

Figure 1. Schematic cross sections of (a) the conventional *p-i-n* *a*-Si:H cell, and (b) the *p*-channel FESCs.

Table 1. Parameters for simulation.

Reflectance at the front side of <i>a</i> -Si:H layer	0.2
Reflectance at the back side of <i>a</i> -Si:H layer	0.8
Absorptance of TCO layer	0.1
Absorptance of dielectric layer	0.0
Thickness of <i>p</i> -type/ <i>n</i> -type layer	200 Å/200 Å
Induced charge density at the interface	$1 \times 10^{13} \text{ cm}^{-2}$
<i>i</i> -Layer thickness	0.3 ~ 0.7 μm
Comb electrode spacing	15 μm ~ 200 μm

the surface. As shown in figure 3, the quantum efficiency for light with short wavelengths is dramatically improved by the use of FESC structure.

Figure 4 shows the energy band diagram along the interface between dielectric and *a*-Si : H for the *p*-channel FESC (see figure 1). In the dark, the conduction edge has a flat energy profile along the interface between the dielectric and *a*-Si : H. In contrast, light irradiation causes a band bending which results in a weak lateral electric field for holes. Hence, photo-generated holes are driven towards the dielectric/*a*-Si : H interface by the vertical strong electric field induced by the gate bias, then turned to the comb electrodes by this weak lateral electric field induced by photo irradiation.

Figure 5 shows the energy band diagrams under the comb electrode with work functions of 5.15 eV and 5.5 eV. In the cell using comb electrodes with 5.5 eV work function, the band is pulled up at the metal/*a*-Si : H interface. Hence, the built-in potential should be

effectively increased, which in turn increases open circuit voltage (V_{OC}) and fill factor (FF). Thus, while improved V_{OC} and FF are expected by the use of comb electrode with large work function for the *p*-channel FESCs, comb electrode with smaller work function is advantageous for the *n*-channel device. The FESCs can take any metals as a top contact electrode instead of TCO at the cost of effective area.

Figure 6 shows the maximum output powers of *a*-Si : H solar cells calculated as a function of the comb electrode spacing. The *n*-channel FESC shows smaller spacing dependence of the maximum output power. Note that while the performance of the *n*-channel FESC is almost comparable with that of the *p*-channel FESC, the performance of the conventional *n-i-p* cell is far inferior to that of the *p-i-n* cell. The maximum output powers for *n*-channel FESCs with comb electrode spacings less than

Figure 2. Energy band diagrams along the vertical centre of the cells for the conventional *p-i-n* cell and the *p*-channel FESC.

Figure 3. Quantum efficiency of the various solar cells.

Figure 4. Energy band diagrams of a *p*-channel FESC along the interface between the dielectric and *a*-Si : H, with and without the light irradiation.

Figure 5. Energy band diagrams under the comb electrode with the work functions of 5.15 eV and 5.5 eV for the *p*-channel FESC.

Figure 6. Maximum output power profiles calculated as a function of the comb front electrode spacing. The *i*-layer thickness for *n*-channel FESC and *n-i-p* junction were assumed to be 0.4 μm , while that for *p*-channel FESC and *p-i-n* junction were 0.6 μm . The FE-induced charge density was set at $1 \times 10^{13} \text{ cm}^{-2}$.

50 μm , are slightly smaller than those for *p*-channel FESCs. This can be attributed to the difference in the type of the carriers which drift in the direction normal to the surface. It is well known that the mobility of a hole in *a-Si:H* is much smaller than that of an electron. Since a large portion of carriers in the *a-Si:H* are generated near the surface, holes in the *n*-channel FESCs must travel long distance, which in turn results in the higher possibility of recombination with the electrons. This difference in the properties of carriers also affect how the dependence of cell performance on such a cell parameter as *i*-layer thickness. We can presume that the optimum thickness of *i*-layer for *n*-channel devices is smaller due to the higher recombination possibility of the photo-generated holes. In fact, the *i*-layer thickness which gives the maximum output power for the *n*-channel FESC is calculated to be about 0.4 μm , while that for *p*-channel FESC is 0.6 μm . While the short hole-drift distance is essentially important for the *n*-channel FESCs, high concentrations of hole-electron pair generation is important for the *p*-channel FESCs.

The *n*-channel FESCs can give a conversion efficiency higher than *p*-channel FESC with prolonged comb electrode spacing. For the FESCs with large comb electrode spacing, the resistance for the lateral motion of the carriers limit the cell performance. In the *n*-channel cells, we can take advantage of high mobility of the electrons in this lateral transportation.

4. Conclusion

The two-dimensional device simulation has shown that both the *n*- and *p*-channel *a-Si:H* FESCs exhibit improved performance compared to conventional cells. This improvement can be explained mainly by the increased quantum efficiency for high energy photons due to the elimination of the heavily-doped window layer. An additional advantage of the FESCs is flexibility in the choice of the metal electrode. To achieve high conversion efficiency, while reduction in the hole-drift distance, i.e. the thickness of intrinsic *a-Si:H* layer, is important for the *n*-channel devices, reduction in the comb electrode spacing is important for the *p*-channel device.

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