Theoretical Analysis of Optimum Bandgap Profile of Cu(In,Ga)Se₂ Solar Cells with

Optical and Defect Properties

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Abstract

The effects of graded bandgap profile on the cell performance of $Cu(In,Ga)Se_2$ solar cell were investigated by device simulator. Optimum bandgap profiles with various defect densities were simulated. In addition, the superiority of the graded bandgap profile was indicated by the comparison with CIGS solar cells without grading.

1. Introduction

The bandgap of Cu(In,Ga)Se₂ (CIGS) is tunable from 1.0 to 1.7 eV by the composition ratio of Ga/(In+Ga), realizing optimum design for solar cell absorbers. Generally, high quality CIGS films were fabricated at high substrate temperature (~550°C), but recently many researchers deposit them at low temperature of below 500°C. The quality of the CIGS films deposited at low temperature should be lower than that deposited at high temperature. However, the high efficiency of 20% was reported in CIGS solar cells based on CIGS films deposited at low temperature, which is realized by the optimization of bandgap profile [1].

On the other hand, the defect densities in CIGS are significantly influenced by the deposition methods such as evaporation, selenization, spin coating, printing, and electrodeposition methods. Therefore, CIGS bandgap profiles with various defect densities are needed to be optimized.

In this study, the optimization of bandgap profile of CIGS solar cells was conducted to show superiority of graded bandgap profile using device simulator, a Solar Cell Capacitance Simulator (SCAPS), which was developed by Gent University [2].

2. Experiment

Solar cell performance was simulated using SCAPS. CIGS solar cell structure in SCAPS was n⁺-ZnO/i-ZnO/ CdS/CIGS. Fig. 1 shows the CIGS bandgap profile and Table I summarizes the device parameters in the simulation. In this Table, E_d is the defect level from E_v , W_d is the defect distribution width, ε_r is the relative permittivity. The positions of Eg₂ were 0.2 µm (inside space charge region (SCR)) and 0.5 µm (outside SCR) from the CIGS surface and each bandgap (Eg) was varied as shown in Table I.

Additionally, in order to show the superiority of graded bandgap profile, the CIGS bandgap profiles with and without grading was compared. For both bandgap profiles, the same generation rate of carrier $(2.1 \times 10^{17} \text{s}^{-1} \text{cm}^{-2})$ was fixed by adjusting Eg.



Fig. 1 Model of CIGS bandgap profile.

Table I Device Parameter in simulation	Table I	Device	Parameter	in	simula	tion.
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Thickness (µm)	2.0	Defect distribution	Gaussian
ε _r	10.0	Defect density (cm-3)	1.0×10^{15} or
N_A (cm ⁻³)	2.0×10^{16}		1.0×10^{16}
N_{C} (cm ⁻³)	2.0×10^{18}	$E_d(eV)$	0.8
N_V (cm ⁻³)	2.0×10^{18}	W _d (eV)	0.1
μe (cm ² V ⁻¹)	100	$Eg_1(eV)$	1.0~1.3
μh (cm ² V ⁻¹)	25	$Eg_2(eV) \cdot Eg_3(eV)$	1.0~1.7

3. Results and discussion

The highest efficiency was achieved with Eg₁ of 1.3eV. Figure 2 depicts solar cell performance map with fixed Eg₁ of 1.3 eV. The best bandgap profiles were independent on the defect density. In the case of X=0.5 μ m, the best bandgap profile was Eg₁=1.3 eV, Eg₂=1.3 eV and Eg₃=1.5 eV. Although this profile did not show the double graded profile, it leads to the highest efficiency because fill factor was decreased by forming grading toward the surface to impede photo-generated electron collection.

In the case of X=0.2 μ m, the best bandgap profile was Eg₁=1.3 eV, Eg₂=1.2 eV and Eg₃=1.5 eV, which is double graded bandgap profile. The photo-generated electrons are efficiently collected in this profile because Eg₂ position is inside SCR. As a result, the decrease in the fill factor was suppressed, thereby resulting in the highest efficiency.



(b) Defect density of 10¹⁶cm⁻³. Fig. 2 Solar cell performance map with fixed Eg of 1.3 eV

The CIGS solar cells with a flat band profile and the double graded bandgap profile are compared in order to reveal the superiority of grading profile. Figure 3 shows (a) current-voltage (I-V) curve and (b) external quantum efficiency (EQE) of the solar cells. The efficiency of the cell with graded bandgap profile was 1.7 % higher than that with the flat bandgap profile. Even though the generation rate of carriers were identical for both profiles, i.e. $2.1 \times 10^{17} \text{s}^{-1} \text{cm}^{-2}$, the short-circuit current density of the cell with the graded bandgap profile was 1.1 mA higher than that with the flat bandgap profile. As shown Fig. 3 (b), the short-circuit current density was increased due to higher carrier collection for long wavelength light. In addition, the open-circuit voltage and fill factor of the cell with graded bandgap profile were higher than those with the flat bandgap profile because recombination at the SCR was reduced by wider bandgap. The results suggest that the grading bandgap profile is useful to obtain high efficiency CIGS solar cells.



Fig. 3 (a) I-V curve and (b) external quantum efficiency of CIGS solar cells with and without Eg grading.

4. Conclusions

The effects of the graded bandgap profile on the cell performance were investigated by SCAPS. When the position of Eg_2 is in SCR, high efficiency was achieved due to the double graded bandgap profile. However, when the position of Eg_2 is outside SCR, the best bandgap profile was not double graded profile because of decreasing fill factor. In addition, the CIGS solar cells with a flat band profile and the double graded bandgap profile are compared. As a result, all solar cell parameter was increased by forming double graded band profile.

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