Simulation-Based Evolutionary Approach to Electrical Characteristic Optimization of *p-i-n* Silicon Thin-Film Solar Cells

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ABSTRACT

Solar cell is one of the most potent candicates for the next-generation energy technology due to its enviromental friendliness and renewable merit. Nowaday the major challenge is to lower fabrication cost while significantly enhancing the energy conversion energy. In this work, a simulator-based optimization for a-Si thin film solar cell with *p-i-n* structure is presented. Using genetic algorithm and electro-optical simulation, running on UOF platform, the optimal designs with respect to energy conversion efficiency, fill factor, short-circuited current density, and open-circuited voltage are obtained. Besides, the sensitivity analyses for different four cases are also conducted to investigate the degradation due to parameter variations. The best overall performance of a single layer a-Si thin film solar cell is achieved with energy conversion efficiency of 7.90% and an average efficiency is 7.35% if considers parameter variations.

Keywords: Amorphous Silicon, Thin-Film Solar Cell, *p-i-n* Structure, Energy Conversion Efficiency, Transport Model, Optical Model, Numerical Simulation, Genetic Algorithm, Simulation-Based, Sensitivity Analysis.

1 INTRODUCTION

Solar cell [1], which can provides renewable and clean energy by converting sunlight to electrical power, is one of the most promising energy technologies in order to relieve the impact of the climate change. Yet, before in replace of fossil fuel for electrical power generation, the fabrication cost of solar cells is urgently to be reduced and the energy conversion efficiency increased significantly. At present, crystalline silicon (c-Si), polycrystalline silicon (poly-Si), and amorphous silicon (a-Si) are the main developed silicon-based materials exploited in solar energy industries. Optimal design of thin-film solar cell in pursuit of high energy conversion efficiency can be reached in a trial-and-error engineering way. On the other hand, genetic algorithm (GAs) is a population-based global searching optimization method based on the mechanism of natural selection, and often considered as the most famous branch in evolutionary algorithms. In theory, GAs with appropriate elitist policy can guarantee the acquirement of the best solution in the global domain and generally can provide many near-optimal selections of the problem. In practice, GAs can provide promising observation and are popularly applied in engineering domains with modification in various types [2]. For a basic *p-i-n* structure of a-Si thin-film solar cell, the efficiency is 5% [1]. Thus, characteristic optimization of a-Si thin film solar cell using GAs is an interesting approach for solar cell technologies.

In this work, a coupled device-optical simulation-based GAs is implemented to optimize electrical properties of a-Si thin-film solar cells under illumination. With numerically solving a set of transport equations in device simulation, the optimal design parameters of explored thin film solar cell can be obtained via genetic algorithm method. The iteration of evolution is terminated once the convergent solution is acquired. The evolutionary technique enables us to optimize the key electrical characteristics, such as short-circuited current (J_{sc}), open-circuited voltage (V_{oc}), fill factor (FF), and energy conversion efficiency (η) of the explored *p-i-n* a-Si thin film solar cell.

2 THIN-FILM SOLAR CELL AND GOVERNING PHYSICAL MODELS

2.1 THE ELECTRICAL MODEL

The basic *p-i-n* structure of a-Si thin film solar cell is illustrated in Figure 1. The silver contact and anti-reflection coating made of Si_3N_4 are deposited over the top surface of a-Si thin film solar cell. In order to investigate the physical characteristic in a-Si thin film solar cells, the governing equations including Poisson equation, current continuity equations, and drift-diffusion model for charge carrier transportation used in the simulation are shown in follows:

$$\nabla \cdot (\varepsilon \nabla \Phi) = -e(p - n + N_D - N_A) - \rho_{trap}, \tag{1}$$

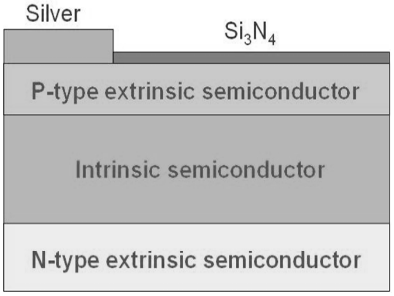
$$\bar{J}_n = e(-n\mu_n \nabla \Phi_n + D_n \nabla n), \tag{2}$$

$$\bar{J}_p = -e(p\mu_p \nabla \Phi_p + D_n \nabla p), \tag{3}$$

$$\nabla \cdot \bar{J}_n = eR_{net} + e\partial_t n + G^{Opt}, \tag{4}$$

and

$$\nabla \cdot \bar{J}_p = -eR_{net} + e\partial_t p + G^{Opt}, \tag{5}$$



Parameters to be optimized of the studied *p-i-n* solar cell

Physical and Structural Parameters	Variables	Range
Thickness of silver contact (μm)	FrontContactThickness	0.05 - 0.3
Thickness of anti-reflection layer (μm)	FrontArcThickness	0.05 - 0.2
Thickness of whole semiconductor (μm)	SubstrateThickness	0.5 - 1.0
Doping concentration of *p*-layer (cm^{-3})	FrontDopingConcentration	10^{19} - 10^{20}
Dopant depth of p-layer	FrontDopingDepth	0.01 - 0.1
Doping concentration of *n*-layer(μm)	BackDopingConcentration	10^{18} - 10^{20}
Dopant depth of *n*-layer	BackDopingDepth (μm)	0.01 - 0.1

Figure 1: A 2D plot of a-Si solar cell with the *p-i-n* structure. The right table lists the parameters to be optimized including numerical ranges.

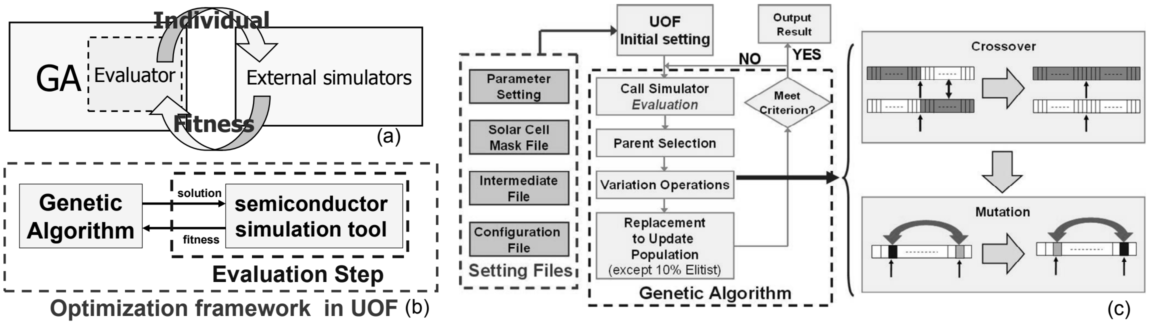


Figure 2: (a) Basic idea of simulation-based GA method. (b) The input/output relationship between GA and semiconductor simulatior. (c) The implemented optimization technique based upon UOF to improve the electrical characteristics of the examined a-Si thin film solar cell.

where ε is the electrical permittivity, e is the elementary electric charge, n and p are the electron and hole densities, N_D and N_A are the concentration of ionized donors and acceptors respectively, ρ_{trap} is the charge density contributed by traps, R_{net} is the net rates of recombination, J_n and J_p are the electron and hole current density. Φ_n and Φ_p are quasi-Fermi potential for n and p. μ_n and μ_p are mobility functions of electrons and holes. D_n and D_p are diffusion coefficients for electron and hole. The optical generation rate, G^{opt},which describes the excitation event of the optical charge carrier under illumination of the standard AM1.5 global spectrum, is coupled into the current continuity equation. Note that herein we assume the optical generation for electrons and holes are pairly produecd.

2.2 THE OPTICAL MODEL

In order to calculate the optical charge carriers generated in a-Si thin film solar cell, a set of Maxwell's equation is considered in the device simulation. Using transfer matrix method (TMM), the optical generation rate G^{opt} can be formulated by solving the following equations:

$$\nabla \times \overline{E} = -\partial_t \overline{B}\,, \tag{6}$$

$$\nabla \times \overline{H} = \overline{J} + \partial_t \overline{D}\,, \tag{7}$$

$$\nabla \cdot \overline{D} = \rho\,, \tag{8}$$

$$\nabla \cdot \overline{B} = 0\,, \tag{9}$$

and

$$G^{Opt} = \alpha \eta I(x) / \hbar\omega\,, \tag{10}$$

where E and D are eletric field intensity and flux density, H and B are magnetic field intensity and flux density, α is absorption coefficiency, η is quantum yield, $\hbar\omega$ is the photon energy. $I(x)$ is the power intensity at the position x in the device, which can be related to:

$$I_{TE,TM}(x) = \frac{\Re(Z_j)}{\Re(Z_0)} \left[\left| \overline{E}^{+}(x) \right|^2 + \left| \overline{E}^{-}(x) \right|^2 \right], \tag{11}$$

$$I(x) = I_{TE}(x) + I_{TM}(x), \tag{12}$$

where $E^{+}(x)$ and $E^{-}(x)$ are forwarding and backwarding electric fields, Z_j is the real part of wave impedance of j layer, Z_0 is the real part of intrinsic impedance.

3 SIMULATION-BASED GENETIC ALGORITHM

Figure 2 indicates the computational flowchart of the proposed optimization technique based on UOF integrating GA methodology [3]. In the mask file and parameter setting file, the design parameters to be optimized are defined for the explored *p-i-n* structure of a-Si thin film solar cell. Primary population, which means the first group of parameter configurations, is initialized randomly by encoding a set of design parameters as gene sequences. In one generation of evolution, all individuals in the population pool are evaluated, and then, according to the definition of fitness, superior individuals survived as the parents. Crossover and mutation operators are two key mechanisms for offspring production. In crossover operator, the gene sequence of an offspring will be inherited from one parent, and the rest will be inherited from another. In mutation operator, genetic variation of each offspring will be triggered in random. The certain proportion of superior individuals in the population pool, which are called elitism policy, is reserved and the other part of the population pool is substituted by the offspring. Iteratively, a new population is established and next generation of evolution starts from evaluation step until the stop criterion are met. The stop criterion used in this work are: (1) Fixed number of generations is reached; (2) The solution with the highest ranking fitness has reached a plateau such that successive iterations no longer produce better results. Herein, η, FF, J_{sc}, and V_{oc} are assigned as fitness in the optimization of the parameter configurations.

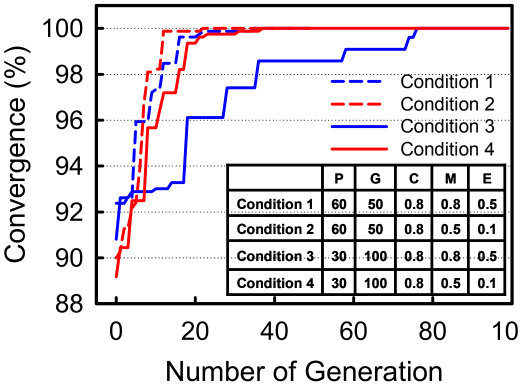


Figure 3: Plot of convergence as function of the number of generations. Settings of four conditions are listed in the inset table.

4 RESULTS AND DISCUSSION

4.1 CONVERGENCE TEST

Figure 3 shows the convergence test as function of the number of generations. Convergence is defined as the best fitness of each generation normalized with respect to the final result. The inset table in Figure 3 indicates the conditions used in the evolutionary simulation. P is the population size, G is the upper limit of generation number, C is the crossover rate, M is the mutation rate, and E is the elitists rate. One can easily find that the globally-explored best solution can be obtained after the 22^{nd} generation of iteration is finished with condition 2. Based on this result, we can set after-30^{th}-generation as the stop criterion in a run to save computation of time. Besides, the convergence can reach a plateau in fewer generations for the condition with large population size than small population size.

4.2 OPTIMAL ELECTRICAL CHARACTERISTICS

Case 1-4 are the optimal electrical characteristics of η, FF, J_{sc}, and V_{oc}. The corresponding design parameters are listed in Table 1. Highest values for η, FF, J_{sc}, and V_{oc} are 7.90%, 88.96%, 8.64mA/cm^2, and 1.1687V respectively. We are concluded that the best overall performance of a-Si thin film solar cell can be achieved with η = 7.90%, FF = 88.40%, J_{sc} = 7.75mA/cm^2, and V_{oc} = 1.1532V.

4.3 SENSITIVITY ANALYSIS

Sensitivity analysis is a dispensable postprocess to assess the stability and reliability of optimal solutions. Considering 10% of optimal structral parameters and 50% of optimal doping concentrations as one standard deviation, a set of randmoly vairated design parameters with respect to the optimal values is generated in Gaussian distribution,and the resulting sensitivity analyses for Case 1-4 are ploted in Figure 4-7. Mean value, normalized standrad deviation, and correlations for Case 1-4 are summarized in Table 2. The analysis shows that the case of optimal efficiency solution is more sensitive to design parameter vairation; instead, the open-circuited voltage is insensitve.

Table 1: The optimized a-Si thin film solar cell structures and electrical performances. Cases 1-4 show optimized characteristic performance of energy conversion efficiency (η), fill factor (FF), short-circuited current density (J_{sc}), and open-circuited voltage (V_{oc}), respectively.

Parameters	Case 1	Case 2	Case 3	Case 4
FrontContactThickness (μm)	0.05	0.20	0.05	0.20
FrontArcThickness (μm)	0.050	0.125	0.050	0.050
SubstrateThickness (μm)	0.50	0.50	1.00	0.50
FrontDopingConcentration	2.75x10^{19}	3.50x10^{19}	4.25x10^{19}	9.5x10^{19}
FrontDopingDepth (μm)	0.10	0.10	0.01	0.10
BackDopingConcentration	6.2x10^{19}	5.8x10^{19}	4.1x10^{19}	7.4x10^{19}
BackDopingDepth (μm)	0.10	0.09	0.06	0.10
η (%)	**7.90**	6.50	6.79	7.27
FF (%)	88.40	**88.96**	79.91	88.47
J_{sc} (mA/cm^2)	7.75	6.40	**8.64**	6.95
V_{oc} (V)	1.1532	1.1423	0.9841	**1.1687**

Table 2: The results of sensitivity analyses for Case 1-4.

		Case 1 (η)	Case 2 (FF)	Case 3 (J_{sc})	Case 4 (V_{oc})
Optimal Electrical Characteristics		7.90%	88.96%	8.64 mA/cm^2	1.1687 V
Mean Value		7.35%	85.07%	8.52 mA/cm^2	1.1392 V
Normalized Standard Deviation		5.38%	3.00%	3.44%	2.56%
Correlation	η	1	0.5016	0.6028	0.1868
	FF	0.9398	1	0.4347	0.7807
	J_{sc}	-0.1819	-0.1168	1	-0.3447
	V_{oc}	0.7675	0.7706	0.1084	1

5 CONCLUSIONS

In this study, an optimization method integrates genetic algorithm and numerical semiconductor simulator is presented for optimal design problem of a-Si thin film solar cell. The objectives are electrical characteristics of a-Si thin film solar cells, and the design parameters are optimized. Also, the sensitivity analyses for optimal solutions are conducted to examine the stability and reliability of electrical characteristics in a-Si thin film solar cells. The excellent performances of the optimization technique not only provide superior structure configurations but also imply that the approach has enough capability to solve other solar cell design problems with more complicated structures, that is, copious variables to be optimized. Currently, we apply this method to optimal design of tandem a-Si thin film solar cells. Furthermore, for the aim of spending less time, distributed computing technique will be considered.

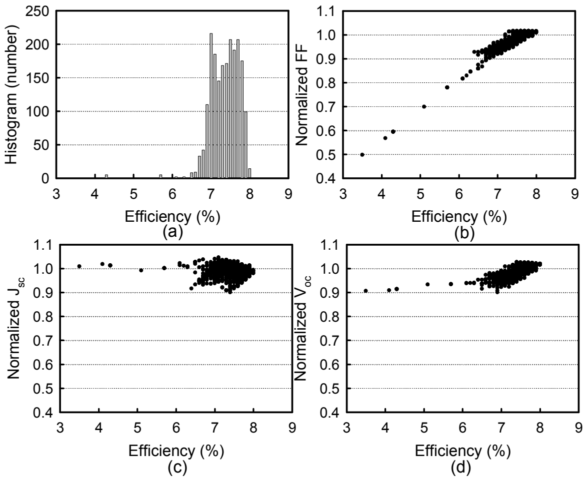


Figure 4: Sensitivity analysis for Case 1. (a) plots the histogram of efficiency. (b)-(d) are the other eletrical characteristics as function of efficienccy.

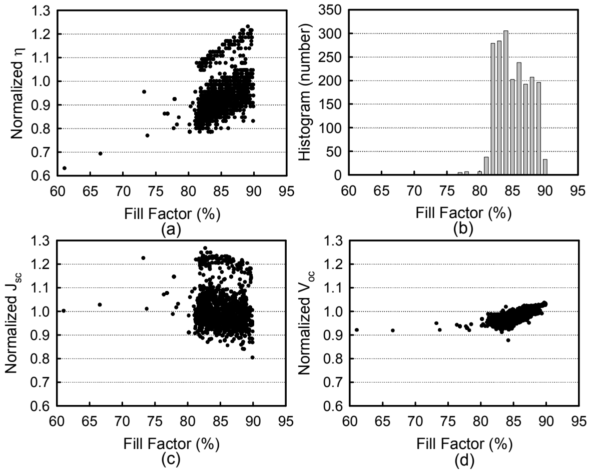


Figure 5: Sensitivity analysis for Case 2. (b) plots the histogram of fill factor. (a), (c) and (d) are the other eletrical characteristics as function of fill factor.

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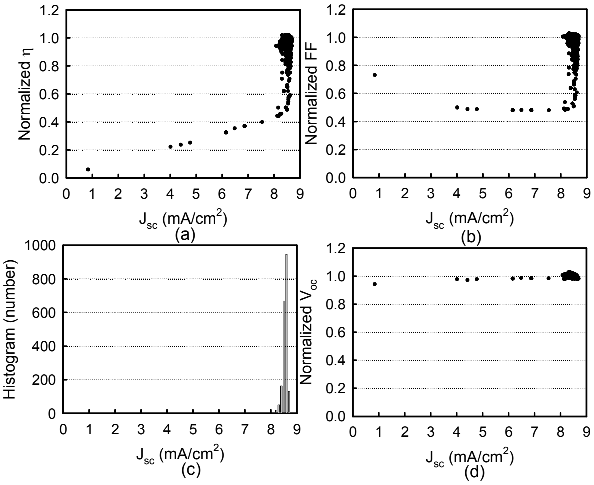

Figure 6: Sensitivity analysis for Case 3. (c) plots the histogram of J_{sc}. (a), (b) and (d) are the other eletrical characteristics as function of J_{sc}.

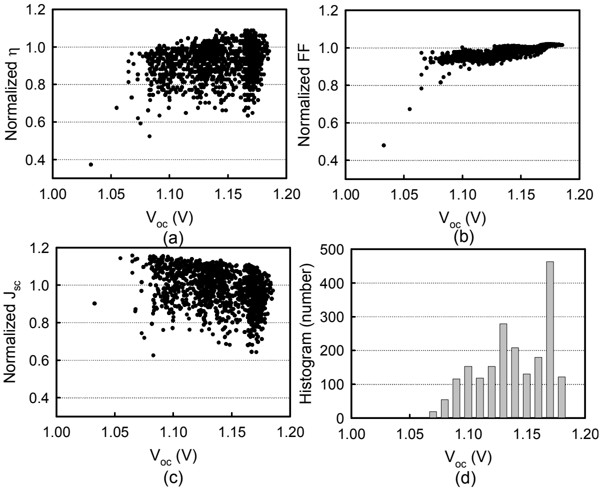

Figure 7: Sensitivity analysis for Case 4. (d) plots the histogram of V_{oc}. (a)-(c) are the other eletrical characteristics as function of V_{oc}.