Opto-Electronics Review 25 (2017) 229–237

Contents lists available at ScienceDirect

Opto-Electronics Review

journal homepage: http://www.journals.elsevier.com/opto-electronics review

A new direction in design and manufacture of co-sensitized dye solar cells: Toward concurrent optimization of power conversion efficiency and durability

M. Hosseinnezhad[a,*], A. Shadman[b], M. Reza Saeb[c,*], Y. Mohammadi[d]

[a] Department of Organic Colorants, Institute for Color Science and Technology, P.O. Box 16656118481, Tehran, Iran
[b] Department of Industrial Engineering, Ferdowsi University of Mashhad, P.O. Box 91775-1111, Mashhad, Iran
[c] Department of Resin and Additive, Institute for Color Science and Technology, P.O. Box 16656118481, Tehran, Iran
[d] Petrochemical Research and Technology Company (NPC-rt), National Petrochemical Company (NPC), P.O. Box 14358-84711, Tehran, Iran

ARTICLE INFO

Article history:

Keywords:
Dye-sensitized solar cell
Co-sensitization
Response surface methodology
Organic dye
Desirability function

ABSTRACT

A novel methodology was implemented in the present study to concurrently control power conversion efficiency (η) and durability (D) of co-sensitized dye solar cells. Applying response surface methodology (RSM) and Desirability Function (DF), the main influential assembling (dye volume ratio and anti-aggregation agent concentration) and operational (performance temperature) parameters were systematically changed to probe their main and interactive effects on the η and D responses. Individual optimization based on RSM elucidated that D can be solely controlled by changing the ratio of vat-based organic photosensitizers, whereas η takes both effects of dye volume ratio and anti-aggregation concentration into account. Among the studied factors, the performance temperature played the most vital role in η and D regulation. In particular, however, multi-objective optimization by DF explored the degree to which one should be careful about manipulation of assembling and operational parameters in the way maximization of performance of a co-sensitized dye solar cell.

1. Introduction

At the present time, the main concern of researchers is to find energy sources with minimum possible contamination toward the environment. Following the pioneering work by O'Regan and Gratzel in 1991 [1], exploration of dye-sensitized solar cells (DSSCs) as environmental-friendly devices capable of generating electron with receive photon from sun light, diverse publications were directed towards improvement of photovoltaic performance of DSSCs manipulating various operational and assembling parameters [2,3]. In general, dye monolayer chemicals were considered to play the role of a material parameter that could govern the performance of DSSCs [4]. In addition, the use of organic dye precursors brought the benefits of low cost and facile dye synthesis, meanwhile a fairly high power conversion efficiency (η) [5,6]. Most of all, it was attempted to synthesize engineering dyes with acceptable light harvesting ability [7], minimum possible aggregation potential [8,9], as well as very low charge recombination tendency [10]. With this aim in view, miscellaneous organic dyes were examined among which are thiophene, indoline, coumarine, and cyanine [11]. Vat based organic dyes are a new class of DSSC sensitizers exhibiting superior thermal, chemical and photochemical resistance [12]. Vat compounds are classified by colour index 10 as dyes and pigments. Indigo and thioindigo and their derivatives are important members of this class. The parent molecules, indigos, are extracted from natural plants, even though their derivatives are mostly prepared industrially. On the other hand, thioindigo does not exist in the nature and has been synthesized over the past century [11,12].

Despite acceptable intensity associated with the use of individual organic sensitizers, the narrow range of absorption of solar spectrum places some limits on their application [13]. This situation has been resolved by introduction of co-sensitization approach, through which η of solar cell has been enhanced significantly [14,15]. Chang et al. fabricated a co-sensitized solar cell (Co-DSSC) and achieved efficiency of 6.70 percent, which was well above values reported for individual DSSCs [16]. Kumara et al. proposed the idea of mixing dyes in a solution containing organic and natural photosensitizers, thereby improved efficiency of Co-DSSCs up to 1.13 percent [17]. Nonetheless, the spectrum range was not still

---

* Corresponding authors.
E-mail addresses: hosseinnezhad-mo@icrc.ac.ir (M. Hosseinnezhad), saeb-mr@icrc.ac.ir (M.R. Saeb).

http://dx.doi.org/10.1016/j.opelre.2017.06.003
1230-3402/

wide enough to warrant a high light harvesting ability responsible for elevating the efficiency. This inability was arisen from disuse of blue hue organic dye in the studied systems.

To the best of our knowledge, there is no report on lab- or industrial- scale production of vat based Co-DSSCs. The merit of vat based organic dyes lies in their low molecular weight, as well as the ability to yield blue hue guaranteeing a wide wavelength interval. Nonetheless, aggregation of vat dyes leading to banned or reduced electron transfer from the exited dye molecules to the photoelectrode should be taken into account when designing Co-DSSCs [18]. From this perspective, it seemed essential to utilize anti-aggregation agents in fabrication of DSSCs. The literature provides useful information on to what extent concentration of anti-aggregation agent governs the η of DSSCs [19]. Since DSSC devices work on the basis of one sun illumination, temperature plays a key role in solar cell performance [20].

Although the importance of η of DSSCs has been noticed by the researchers and engineers alike, a few reported on durability (D) of such devices, in spite of its vital importance from an application point of view. Takada et al. [21] and Lin et al. [22] noticed some points to improve D of DSSCs. Accordingly, it was found that utilization of carbon as working electrode or Pt as counter electrode improves the D of DSSCs. Nonetheless, available reports still lack a complete view on how D of DSSCs can be optimized by manipulating operational and assembling variables. An alternative method would be application of Co-DSSCs in which two vat-based organic dyes are mixed together and applied directly instead of sequentially. In a previous work we reported on enhancement of cell efficiency when using two dyes with respect to the case each dye was applied [23]. Nevertheless, the role of assembling and operating parameters has not been studied.

In the present work, we systematically changed volume ratio of dyes, performance temperature, and concentration of Cheno anti-aggregation agent to fabricate a series of Co-DSSCs to control η and D of Co-DSSCs using Response Surface Methodology (RSM) and Desirability Function (DF). Such combinatorial approach has been successfully applied by others for solving different multi-criteria optimization problems [24–26]. On the basis of RSM, volume ratio of vat-based organic dyes in a binary dye solution, concentration of anti-aggregation agent, and performance temperature were changed systematically, as explanatory variables, to enable concurrent control of η and D of Co-DSSCs. Of note, the idea of manufacturing Co-DSSCs with maximum attainable η and D has been disclosed here for the first time. Statistical analyses based on first-order, first-order with interaction, and second-order regression functions provided a detailed information about dependency of Co-DSSCs on performance temperature, which is the key finding of this work. Multi-objective optimization of the aforementioned targets by DF approach draws a new direction in identifying the individual and interactive effects of assembling and operational variables on η and D of Co-DSSCs.

2. Experimental design and statistical analyses

All ingredients used in synthesis and preparation of solar cells were analytical grades provided by Merck Co. and used as received. The two organic dyes, hereafter referred to as Dye 1 (indigo dye) and Dye 2 (thioindigo dye), innovatively synthesized and fully characterized in our previous papers were also used without further treatment [12,27]. These organic dyes were manufactured on the basis of indoxyl and thioindoxyl, respectively, through standard reactions and purified. Different mixtures of the assigned dyes were applied in production of Co-DSSCs.

To investigate the performance of manufactured Co-DSSCs, action spectra corresponding to each device were measured under monochromatic light with a constant photon number (5×10^{15} photon cm^{-2} s^{-1}). Photocurrent-photovoltage (J-V) characteristics of devices was measured under illumination with AM 1.5 simulated sun light (100 mW cm^{-2}) through a shading mast (5.0 mm × 4 mm) by using a Bunko-Keiki CEP-2000 system.

Table 1
Experimental range and coded levels of independent variables.

Variable	Symbols	Unit	Ranges and levels		
			−1	0	1
Volume of Dye1	A	(mL)	0	2.5	5
Performance-temperature	B	(°C)	10	30	50
Concentration of anti-aggregation agent	C	(mM)	0	10	20

In the light of previous studies, three explanatory variables including volume ratio of organic dyes (Dye 1/Dye 2), concentration of anti-aggregation agent, and performance-temperature were selected, as the most influential factors governing the η and D of DSSCs, and changed (Table 1). Since total volume of dye mixtures was unconditionally kept constant at 5 mL, we detected variations in η and D as a function of Dye 1 vol. Obviously, the volume of Dye 2 in the mixture can be simply calculated subtracting volume of Dye1 by total volume of 5 mL.

Application of RSM enabled systematic evaluation of the effects of chosen assembling and operational parameters, nominated as A, B, and C in Table 1, on the η and D of Co-DSSCs.

In general, first and second-order regression functions are suitable for analyzing the problem of interest, as follows [28]:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots\ldots\beta_k x_k + \varepsilon \qquad (1)$$

$$y = \beta_0 + \sum_{j=1}^{k} \beta_j x_j + \sum_{j=1}^{k} \beta_{jj} x_j^2 + \sum \sum_{i<j=2}^{k} \beta_{ij} x_i x_j + \varepsilon. \qquad (2)$$

In the above formulas, x and y are indicative of changing and response variables, respectively. Approximating functions take noises or errors in prediction of response variable into account in terms of ε in Eqs. (1) and (2). The coefficients β_1, β_2, . . ., and β_k in Eq. (1) take the main effects of changing variables on the selected response variable (in the current work η or D), while coefficients β_{jj} and β_{ij} in Eq. (2) are known as curvature and interaction terms reflecting the interactive effects between changing variables, respectively. When one has aimed at investigating the interaction between changing variables, quadratic interpolation function could provide more information about actual effects of parameters [29–32].

According to variation levels proposed by RSM, fifteen solar cells were manufactured and their η and D were measured and tabulated. Based on three-factor Box-Behnken Design (BBD), fifteen experiments were designed as represented in Table 2. Design Expert software package version 7 was used for design analysis and optimization.

In case of RSM, three types of regression functions were applied to experimental data: (*i*) linear model; (*ii*) linear model with interactions; and (*iii*) quadratic model. The coefficient of determination (R-squared or R^2) and adjusted R^2 (Adjusted-R^2) were compared in each case to indicate which model brings more precision among all studied models. In addition, depending on the selected response, the reduced form of the regression function was considered through which a better fit was obtained. Accordingly, we realized which factors, independently or simultaneously affect the η and D target variables.

The set of optimal solutions was obtained, in the second step of optimization, with the aid of multi-criteria optimization by DF