Chapter 15

Parameter Estimation in Organic-Based Schottky Diodes Used in Solar Cell Applications with Artificial Intelligence Optimization Algorithms

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Abstract

The electrical characterization of organic semiconductor materials plays a critical role in the design of advanced electronic devices and the understanding of their performance. Particularly, electrical parameters such as the ideality factor, barrier height, and series resistance, derived from the current-voltage (I–V) characteristics of rubrene-based metal-polymer semiconductor (MPS) structures, provide fundamental insights into the material's intrinsic and interfacial properties. The nonlinear nature of these parameters and the uncertainties associated with experimental data render traditional estimation methods inadequate. Additionally, investigating the effects of external factors, especially Cobalt-60 gamma irradiation, on these electrical parameters is of great importance for device reliability. The aim of this study is to accurately and reliably estimate the electrical parameters of Al/rubrene/p-Si Schottky-Junction solar cell using Artificial Intelligence (AI) optimization algorithms, based on experimental I–V data obtained after Cobalt-60 gamma irradiation. In this context, a total of twelve different AI optimization algorithms were employed, including Genetic Algorithm, Differential Evolution, Flower Pollination Algorithm, Artificial Bee Colony, Ant Colony Optimization, Bat Algorithm, Cuckoo Search Algorithm, Grey Wolf Optimization, Jaya Algorithm, Particle Swarm Optimization, Harmony Search, and Teaching-Learning-Based Optimization. The estimation of electrical parameters was performed using I–V measurements conducted across five different

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forward voltage ranges, with the performance of the algorithms evaluated using *MAPE* and R^2 metrics. This study presents that the AI optimization algorithms can be used as optimization tool for parameter estimation of Schottky diode model and the algorithms may offer more effective results compared to traditional optimization methods in the electrical analysis of organic semiconductor models under Cobalt-60 irradiation.

INTRODUCTION

In the contemporary scientific landscape, the accurate modelling of complex systems has become a prevalent necessity. This has prompted researchers to adopt more flexible modelling approaches that transcend linear assumptions. In this context, the employment of nonlinear models becomes important, particularly in scenarios where the relationships between variables cannot be satisfactorily explained linearly. The nonlinear regression models are powerful statistical tools used when the relationships between dependent and independent variables are parametrically nonlinear. These models enable a more realistic and reliable representation of real-world phenomena across a wide range of disciplines, including engineering, economics, biomedical sciences, environmental sciences, and social sciences. However, the mathematical complexity introduced by the nonlinear structure presents significant challenges, particularly in the parameter estimation process, and limits the effectiveness of classical methods (Gallant, 1975).

Parameter estimation of nonlinear regression models is generally formulated as an optimization problem based on the minimization of the sum of squared errors. Traditional optimization methods used in this process, such as Gauss-Newton, Levenberg-Marquardt, and other derivative-based methods, may yield successful results under certain conditions (Türkşen, 2023). Nevertheless, they are limited by several issues, including the non-differentiability of the objective function, the presence of multiple local minima, high sensitivity to initial parameter values, and inefficiency in high-dimensional search spaces. In this regard, the challenges encountered in parameter estimation are not only technical but also significant in terms of computational efficiency and model reliability.

These limitations are especially important in solar cell modelling, which is becoming more and more important because of its role in condensed matter physics and its importance in the development of efficient photovoltaic structures. Addressing these computational challenges is essential for accurately modeling solar cells, which are key to meeting the global demand for clean and sustainable energy. By converting sunlight directly into electricity without emitting greenhouse gases, these systems represent a promising and environmentally friendly alternative to conventional fossil fuel–based energy sources. To investigate these systems in greater detail, Schottky diodes with an Al/p-type Si structure were utilized. These diodes were fabricated using boron-doped single-crystal silicon wafers (p-type) as the semiconductor substrate, onto which aluminum was thermally evaporated to form the Schottky contact. The resulting devices were employed to examine the electrical characteristics and interfacial properties of the metal–semiconductor junction, with the aim of enhancing our understanding of charge transport mechanisms that are crucial for improving photovoltaic performance. Accordingly, this study outlines the fabrication process and electrical characterization of an Al/Ru/p-Si Schottky diode constructed on a p-type (111) silicon wafer. All electrical measurements were performed using a microcomputer-assisted setup through an IEEE-488 compatible AC/DC converter card, ensuring precision and repeatability. The analysis of the electrical behavior was carried out based on the thermionic emission theory, which serves as a foundational framework for evaluating metal-semiconductor and metal-organic semiconductor junctions. The thermionic emission theory provides a quantitative description of how charge carriers primarily electrons exceed the potential energy barrier at the metal-semiconductor interface through thermal excitation. This model enables the measurement of critical diode parameters, like the barrier height, ideality factor, and saturation current. This is important for seeing how well Schottky diodes and other optoelectronic and microelectronic devices work. Furthermore, the thermionic emission theory becomes particularly significant in cases where interface-related effects such as localized states, barrier inhomogeneities, and thin interfacial layers play a substantial role in charge transport. Deviations from ideal thermionic emission behavior under these conditions can reveal the presence of interface traps, tunneling mechanisms, or spatial variations in barrier height. Understanding and quantifying these non-idealities are essential for optimizing device architecture, especially in advanced applications including harsh or radiation-exposed environments.

In metal-organic semiconductor Schottky barrier diodes, the barrier height has also been shown to exhibit voltage dependence, further complicating the transport dynamics and necessitating more detailed modeling approaches that incorporate both intrinsic and extrinsic influences on charge flow. The thermionic emission theory (Sze, 1981) predicts that the current–voltage (I–V) characteristics as in the studies (Akay et al. 2019, Akay et al. 2020, Akay et al. 2024)

In recent years, new methods inspired by nature and human behaviour have been developed to overcome these challenges. In particular, computer programmes that optimise things have been shown to be a good option for nonlinear regression analysis. The AI optimization algorithms, called Genetic Algorithm (GA), Differential Evolution (DE), Flower Pollination Algorithm (FPA), Artificial Bee Colony (ABC), Ant Colony Optimization (ACO), Bat Algorithm (BA), Cuckoo Search Algorithm (CSA), Grey Wolf Optimization (GWO), Jaya Algorithm (JA), Particle Swarm Optimization (PSO), Harmony Search (HS), and Teaching-Learning-Based Optimization (TLO), stand out with their ability to effectively explore large search spaces, significantly overcoming the local minimum traps encountered by traditional algorithms. Moreover, these algorithms operate without requiring derivative information and are well-suited for parallel processing, thereby demonstrating high computational performance even with large datasets. Numerous studies in the literature have shown that AI optimization algorithms are better than traditional methods because they are more accurate and faster (Açıkgöz, 2025).

The main aim of this study is to comprehensively investigate the applicability of AI optimization algorithms in addressing the parameter estimation problem encountered in nonlinear regression models. In this study, twelve AI optimization algorithms were applied on a parametrically structured nonlinear model called Schottky diode model. Each algorithm's performance was comparatively analyzed in terms of error metrics (*MAPE* and R^2), computation times, and solution stability. The rest of the paper is organized as follows. Nonlinear regression model of Schottky diode and applied AI optimization algorithms are explained in Materials and Methods section. The analysis results are presented in Results section. Finally, conclusion is given in the last section.

MATERIAL AND METHODS

Material

Nonlinear regression models are powerful statistical tools that provide more realistic and reliable results in situations where the assumption of a linear relationship between dependent and independent variables is invalid. (Akgün, 2018). The general form of a nonlinear regression model can be expressed as,

$$Y_i = f\left(\boldsymbol{X}_i, \hat{\boldsymbol{a}}\right) + \varepsilon_i \quad , \quad i = 1, 2, \ldots, n \tag{1}$$

where, Y_i represents the dependent variable, $\boldsymbol{X}_i$ denotes the vector of independent variables, $\hat{\boldsymbol{a}}$ is the parameter vector to be estimated, and ε_i is the error term with zero mean and constant variance. The objective of the model is to determine the parameter vector $\hat{\boldsymbol{a}}$ in such a way that the model output best fits the observed data (Khuri and Cornell, 1996). These parameters are estimated numerically by minimizing an objective function based on the sum of squared errors

$$\min \varphi(\boldsymbol{\beta}) = \sum_{i=1}^{n}\left[Y_i - f\left(\boldsymbol{X}_i, \boldsymbol{\beta}\right)\right]^2 . \tag{2}$$

According to the optimization model given in equation (2), the nonlinear *f* function is defined for the electrical characterization of organic semiconductor materials as follow

$$I = I_0 \exp\left(\frac{qV_0}{nkT}\right)\left[1 - \exp\left(\frac{-qV_0}{nkT}\right)\right] . \tag{3}$$

Here, q is an electron charge, k is the Boltzmann's constant, T is an absolute temperature, n is the ideality factor, I_0 is a reverse saturation current and is equal to $A^{*}T^2 \exp\left(\frac{-q\Phi_b}{kT}\right)$ in which Φ_b is a barrier height, A^* is a Richardson Constant. And also, $V_0 = V - IR_s$, where R_s is a series resistance and V is considered as an input variable while the output variable called I, presented in equation (3). In this study, it is aimed to estimate the key electrical parameters n, R_s and Φ_b of Schottky-barrier solar cells with an Al/rubrene/p-Si structure. Here, parameter vector is defined as $\hat{\boldsymbol{a}} = \left[n \ \mathrm{R}s \ \ \Phi_b\right]$. Directly estimating the parameter vector $\boldsymbol{\beta}$ from experimental data is highly challenging due to measurement because of the Cobalt-60 gamma radiation uncertainties. At this point, the AI optimization algorithms offer a more reliable alternative to traditional methods, thanks to their derivative-free nature, robustness against initial conditions, and ability to navigate complex landscapes with multiple optima.

In this study, twelve different AI optimization algorithms were applied to the I–V data derived from the described model. Each AI algorithm was assessed for its ability to accurately and consistently estimate the model parameters. These algorithms utilize heuristic strategies in their solution search processes, enabling them to reach both global and local optima. As such, this approach offers not only high accuracy but also computational efficiency and stability, thereby establishing a robust modeling framework.

Methods

The Collection of the Data

The following experimental sets out the fabrication process of an Al/Ru/p-Si Schottky diode on a p-type (111) silicon wafer, with a thickness of 280 μm and a resistivity of 10 Ω·cm. The wafer was initially subjected to a thorough cleansing process employing the RCA chemical cleaning method. Detailed information about experiment can be seen in the studies of Akay et al. 2019, Akay et al. 2020, Akay et al. 2024. All measurements were conducted with the assistance of a microcomputer via an IEEE-488 AC/DC converter card. The relationship between input (V) and response (I) values can be seen in Figure 1. It can be easily said from Figure 1 that the input and the response values have nonlinear relationship.

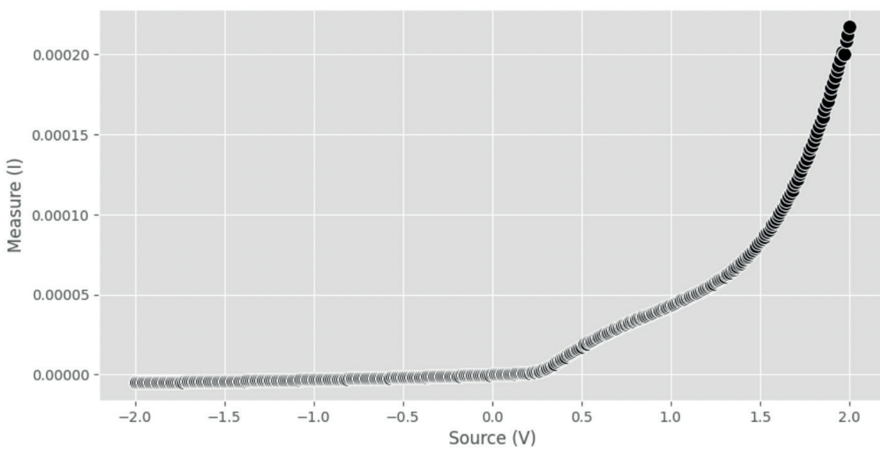

Figure 1. The relationship of input (V) and response (I) values

Statistical Analysis

In this study, the parameter estimation process of a nonlinear electrical model based on experimentally obtained current-voltage (I–V) data was carried out using AI-based algorithms, rather than traditional derivative-based optimization methods. Due to the nonlinear nature of $\boldsymbol{\beta}$ as well as the inherent uncertainties in the measurement data, classical methods often fail to provide reliable estimations. These types of problems typically involve a complex solution space with multiple local minima and are highly sensitive to initial values. Thus, the AI optimization algorithms, inspired by various disciplines, were used in this study. These algorithms are heuristic approaches derived from nature, social behavior, or learning processes and aim to reach higher-quality solutions through an evolutionary process, starting with a numerical population. Each algorithm evaluates candidate solutions searching the problem space based on its internal mechanism, improves them, and generates new candidates to reach the optimal solution. Generally, an initial population of randomly generated individuals is created, followed by information exchange and variation operations among selected individuals. This process iteratively continues to enhance the quality of the solutions step by step. A general working schema of the AI optimization algorithms is presented in Figure 2.

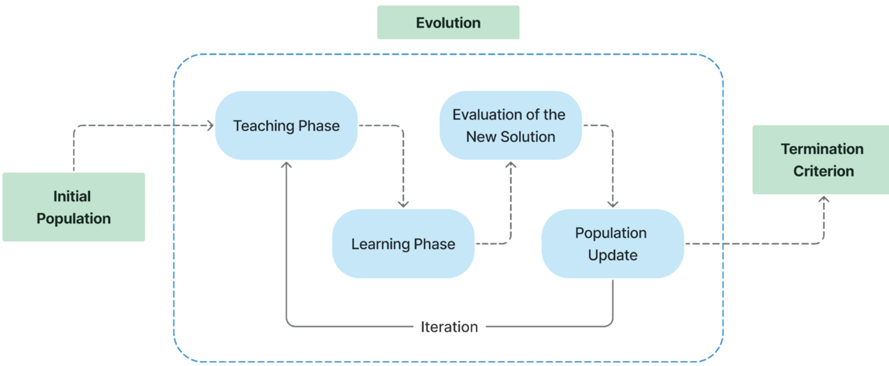

Figure 2. A general schema about working principles of the AI optimization algorithms

Each of these algorithms has been configured to perform parameter estimation for the model built on experimental I–V data, with tuning parameters, carried out for the problem at hand. This process involved optimizing tuning parameters such as population size, number of iterations, crossover rates, learning coefficients, and other control variables to maximize each algorithm's performance. Thus, each algorithm was enabled to function in the most efficient manner appropriate to its structure.

In this study, twelve AI algorithms have been applied in a comparable manner with the aim of minimizing the error function. The tuning parameter values of each AI algorithms are defined by using data-driven expert knowledge and commonly used in the literature. Through the *MAPE* and R^2 metrics, the relative performance of each AI algorithm in terms of accuracy and stability is analyzed. This methodological approach not only enhanced the accuracy of parameter estimation but also provided a robust framework for how AI optimization algorithms can be effectively applied to complex engineering-based modeling problems. In modeling the electrical behavior of electronic structures exposed to external factors such as radiation, these flexible and data-driven optimization approaches offer significant potential for both academic research and industrial applications.

RESULTS

This study aimed to estimate the electrical parameters of Al/rubrene/p-Si Schottky-barrier solar cells after exposure to Cobalt-60 gamma irradiation within the framework of a nonlinear model with minimum error. The optimization results are presented in Table 1. It can be said from Table 1 that the ABC, the DE and the TLO have better performance according to the R^2 metric. The ACOR has the best performance for computing time. It is seen from the results that model parameters estimation is achieved by using the AI optimization algorithms.

Table 1. Optimization results of the AI algorithms with model parameters estimation

AI	Iteration Number	Total Working Time	Iteration Time	*Performance metrics*		*Model parameters estimation*		
				MAPE	R^2	Φ_b	n	R_s
ABC	93	1.3182	0.0126	0.330466	**0.702430**	0.672212	5.000	100.00
ACOR	67	**0.3007**	**0.0034**	0.332134	0.694962	0.672283	5.000	41.31
BA	32	0.5016	0.0046	0.597449	0.395611	0.696066	4.547	45.64
CSA	16	0.7185	0.0069	0.342103	0.666398	0.674036	4.878	54.19
DE	56	0.6041	0.0059	0.330466	**0.702430**	0.672212	5.000	100.00
FPA	86	0.6742	0.0064	0.333669	0.699231	0.672529	4.988	88.39
GA	99	0.7695	0.0075	0.437047	0.641893	0.683048	4.650	99.69
GWO	100	0.6316	0.0062	0.330507	0.702430	0.672215	5.000	100.00
HS	72	0.6773	0.0065	0.348827	0.691971	0.673716	4.960	65.67
JA	8	0.5124	0.0049	0.338779	0.695660	0.672702	5.000	43.80
PSO	38	0.6175	0.0073	0.330492	0.702430	0.672214	5.000	100.00
TLO	51	1.3489	0.0135	**0.330466**	**0.702430**	0.672212	5.000	100.00

These results show that the AI optimization algorithms used in the study not only cover a broader range of parameter values compared to classical methods but also offer more reliable estimations with lower error and higher explanatory power. This highlights the applicability of the AI optimization algorithms in the electrical characterization of organic semiconductor structures, demonstrating significant advantages over classical analytical approaches in terms of accuracy, flexibility, and computational efficiency.

DISCUSSION AND CONCLUSION

In this study, a comprehensive analysis was conducted by integrating nonlinear regression models with the AI optimization algorithms for the electrical characterization of organic solar cells. The results not only revealed the effects of Cobalt-60 gamma irradiation on device performance but also demonstrated that electrical parameters derived from experimental data can be accurately and reliably estimated. The nonlinear modeling approach effectively represented complex system behaviors that are difficult to explain using classical methods, clearly revealing the changes in key parameters, presented as $\boldsymbol{\beta}$.

The AI optimizaton algorithms not only provided balanced performance in modeling but also introduced flexibility into the parameter estimation process by overcoming the limitations associated with traditional techniques. Through AI-based methods, efficient exploration of wide search spaces became feasible, and the derivative-free structure enhanced the generalizability of the modeling process. The findings demonstrate that the AI optimization algorithms offer a robust alternative for analyzing organic electronic devices operating under environmental stress conditions, such as radiation. In this context, AI optimization algorithms are considered applicable to industrial scenarios, particularly for real-time parameter estimation and device performance monitoring.

In conclusion, this study demonstrates the effectiveness of AI-supported parameter estimation processes for both academic research and industrial applications and provides a solid methodological foundation to guide future work in this field.

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Conflict of Interest

The authors have declared that there is no conflict of interest.

Author Contributions

Murat Açıkgöz: Writing – original draft, review & editing, Statistical Analysis, Methodology, Investigation, Interpretation

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