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Optimization of Base Energy Resolution in Hemispherical Deflector Analyzer by using Genetic Algorithm

Murat İnce^{1*}, Nimet Işık²

¹ Vocational School of Technical Sciences, Isparta University of Applied Sciences, Isparta, Turkey ² Mathematics and Science Education Department, Burdur Mehmet Akif Ersoy University, Turkey *<u>muratince@isparta.edu.tr</u> *Orcid No: 0000-0001-5566-5008

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Abstract

The aim of this study is to demonstrate the Genetic Algorithm (GA) optimization results for energy resolutions of the Hemispherical Deflector Analyzer (HDA). The HDAs are designed specifically to distinguish electrons according to their energies. In this context, high energy resolutions are important for the prevention of experimental data loss. Thus, the energy resolution values can be obtained in a short time with the aid of the genetic algorithm implemented in the proposed software. Genetic algorithm (GA) is an effective method developed with artificial intelligence technology. For the first time, analyzer resolution values in the widest range in the literature were calculated by genetic algorithm software. Optimum solutions not only for centric entry HDA but also for paracentric entry Hemispherical Deflector Analyzer (HDA) were obtained by the genetic algorithm.

Keywords: Artificial intelligence, electron optics, electrostatic energy analyzer, genetic algorithm, optimization.

1. Introduction

Energy resolution studies are investigations aimed at increasing the resolution of energy analyzers used in a wide range of fields, from atomic and molecular physics to medical physics [1]. An ideal energy analyzer with high resolution means that the detector located at the analyzer output can better represent, solve, and distinguish different energetic charged particles. The numerically calculations to determine the energy resolution of hemispherical deflector analyzer dates back to the results by Kuyatt and Simpson [2] in the late 1960s, but novel methods of producing fast and effective solutions remain important today. Energy profiles of transmitted particles and variation of the observed energy resolution of an HDA with mean kinetic energy are given by Imhof et al. [3]. It has been proposed to improve the energy resolution of charged particles analyzed by slowing down in subsequent studies [4-7]. Benis and Zouros [8] first showed that the energy resolution of an HDA can be improved by displacing the HDA input to a new position from the conventional position of R (mean radius). With this method, called with paracentric entry HDA, high energy resolution has been achieved [9,10]. The computational results of base energy resolution as a the function of beam entry

diameter are given by Sise et al. [11]. These calculations are carried out by the electron ray-tracing program SIMION which uses the finite difference method [12]. The basic parameters used to determine the energy resolution are dispersion, magnification M and deviation coefficients. For this reason, the calculation values obtained for the different configurations of these parameters are also given by Sise et al. [13]. In these studies, the energy resolution is calculated for some values of parameters. Although these studies in the literature are successful, they need an appropriate dataset to predict an unknown data with high accuracy. Moreover, some of these studies require a training dataset. In this study, the energy resolution is calculated for a wide range of parameter values to get a dataset for future studies without any previously known data.

The aim of this study is the investigation of optimum base energy resolution of the centric and paracentric entry HDA using the genetic algorithm. GA is an artificial search algorithm based on the mechanics of biological evolution [14]. The GA is used widely for many search and optimization problems such as science, business, engineering and education areas [15,16]. In physics, GAs is used for irreversible radiative-type heat engine optimization [17] and lithium-ion battery model optimization [18]. Similarly, in this study, the GA is



used effectively to optimize the base energy resolution of the hemispherical deflector energy analyzers over a wide range of parameters. The energy resolution equation has many parameters in a wide range of values. Thus, the GA is useful for these types of equations to get optimum values in a fast and simple way.

This study consists of three basic parts: In Section 2, the energy resolution of the HDA and the genetic algorithm explained. Section 3 gives the results of the proposed method. The last section concludes the study.

2. Material and Methods 2.1. Base Energy Resolution of Hemispherical Deflector Analyzer

The HDA base energy resolution is related to the maximal beamwidth of electrons. It is defined as the full width of the energy transmission function. The base energy resolution of HDA is given by

$$\frac{\Delta E}{E} = \frac{\Delta r_{\pi} - M\Delta r_0}{D} - \frac{P_1}{D}\alpha - \frac{P_2}{D}\alpha^2$$
(2.1)

Here, *M* and *D* represent the analyzer magnification, and energy dispersion, respectively. P_1 and P_2 stand for the angular aberration coefficients. Δr_0 stands for the beamwidth of the analyzer entry and Δr_{π} represent the exit beam width for the hemispherical deflector analyzer. Boundaries of these parameters are as follow; $0 < \alpha < 5$, $0 < \Delta r_{\pi} < 2$, $0 < \Delta r_0 < 2$, -2 < M < 4, 100 < D < 500, -250 $< P_1 < 250$ and $-250 < P_2 < 250$.

2.2. Basic Principles of the Genetic Algorithm Method

A genetic algorithm is a heuristic optimization and search method to find the best solutions for many problems [19]. As an evolutionary algorithm, the GA is inspired by evolutionary genetics in biology. Inheritance, mutation, selection, and crossover are fundamental components of the GA [20]. The basic steps of the GA are shown in Figure 1. Firstly, the population is initialized with random chromosomes. Then, according to the fitness function, each individual chromosome is evaluated. Best fitted chromosomes are selected to the new population. Selected chromosomes are reproduced by crossing over and mutated [21]. Thereafter, the new population is exposed to the new iteration. When the maximum number of generation count or termination conditions is reached, the GA is stopped [22]. The GA is used for many optimizations, search, and selection problems. The best parameters of components, arrangement, pinch, and approach point are obtained by optimization of a heat recovery steam generator [23]. In Askarzadeh's study [24], power generation in a Microgrid is optimized for minimization of the energy production cost in the smart grid framework. In another study, optimal sensor placement is obtained for the construction of accurate strain maps for large-scale structural components [25]. Armaghani

et. al. [26] make airblast prediction to minimize or reduce the environmental effects of overpressure. In another study, the electrical power load is forecasted to balance the electricity supply and demand [27].



Figure 1. Flow chart of genetic algorithm.

3. Results and Discussion

The proposed GA is used to find a base energy resolution of HDA using Equation (2.1).

- 1. The initial population is generated. α , Δr_{π} , Δr_0 , M, D, P₁ and P₂ that are variables in base energy resolution equation which are encoded as a chromosome with real numbers according to the boundaries (Figure 2). In this encoding, each chromosome is regarded as a candidate solution CS_1 to CS_n where n is population size. CS_1G_1 to CS_nG_1 are genes that represent α , CS_1G_2 to CS_nG_2 are genes that represent, Δr_{π} , CS_1G_3 to CS_nG_3 are genes that represent Δr_0 , CS_1G_4 to CS_nG_4 are genes that represent M, CS_1G_5 to CS_nG_5 are genes that represent D, CS_1G_6 to CS_nG_6 are genes that represent P_1, CS_1G_7 to CS_nG_7 are genes that represent P_2 .
- 2. In Equation (2.1), $\frac{\Delta E}{E}$ is expected to be have a maximum value. Therefore, the fitness function which is to be minimized is founded as:

$$F(x) = 1 / \left(\frac{\Delta r_{\pi} - M\Delta r_0}{D} - \frac{P_1}{D} \alpha - \frac{P_2}{D} \alpha^2 \right)$$
(3.1)



- 3. Calculate the initial chromosome population according to the F(x) fitness function. Then, using the election rate, the best chromosomes that minimize the F(x) are selected to the new population (Figure 3). After, new chromosomes are regenerated and mutated by the mutation rate. The population size was 100, the mutation rate was 0.25, the election rate was 0.15, and the maximum generation count (ε) was 1000.
- 4. When the maximum generation count (ϵ) is reached, GA is finished. The best chromosome in the last

population is shown as the base energy resolution of the HDA (Figure 4). In Fig. 5, the genetic algorithm solutions for the M versus P₁ and P₂ values for $\alpha=0^{\circ}$, $\Delta r_{\pi}=0$, $\Delta r_0 = 1.97$, D=100 mm are given. Although the variation of energy resolution parameters has been examined using different methods in the literature [10,11], for the first time in the literature, the variation of these parameters in Fig. 5 is given in detail, to the best of our knowledge.

		0<α<5	$0 < \Delta r_{\pi} < 2$	$0 < \Delta r_0 < 2$	-2< <i>M</i> <4	100 <d<500< th=""><th>$-250 < P_1 < 250$</th><th>-250<p2<250< th=""></p2<250<></th></d<500<>	$-250 < P_1 < 250$	-250 <p2<250< th=""></p2<250<>
CS_1	\rightarrow	CS_1G_1	CS_1G_2	CS_1G_3	CS_1G_4	CS_1G_5	CS_1G_6	CS_1G_7
CS_2	\rightarrow	CS_2G_1	CS_2G_2	CS_2G_3	CS_2G_4	CS_2G_5	CS_2G_6	CS_2G_7
•	\rightarrow	•	•	•	•	•	•	•
•	\rightarrow	•	•	•	•	•	•	•
•	\rightarrow	•	•	٠	•	•	•	•
•	\rightarrow	•	•	•	•	•	•	•
•	\rightarrow	•	•	•	•	•	•	•
<i>CS</i> _n	\rightarrow	$CS_{n}G_{1}$	$CS_{n}G_{2}$	$CS_{n}G_{3}$	$CS_{n}G_{4}$	$CS_{n}G_{5}$	$CS_{\rm n}G_6$	$CS_{n}G_{7}$

Figure 2. Encoded chromosomes and their boundaries for base energy resolution optimization.



Figure 3. Fitness function values that is to be minimized.



Figure 4. Base energy resolution values that is to be maximized.

The computation results are obtained with the genetic algorithm for the HDA. The calculations are performed using Equation (1) according to $0 < \alpha < 5$, $0 < \Delta r_{\pi} < 2$, $0 < \Delta r_0 < 2$, -2 < M < 4, 100 < D < 500, $-250 < P_1 < 250$ and $-250 < P_2 < 250$. For this context, comparison of M versus P_1 and P_2 values for $\alpha=0^\circ$, $\Delta r_{\pi}=0$, $\Delta r_0 = 1.97$, D=100 mm are given in Figure 5. Moreover comparison of M versus P_1 and P_2 values for $\alpha=0^\circ$, $\Delta r_{\pi}=0$, $\Delta r_0 = 1.97$, D=100 mm are given in Figure 6. Considering the results, the GA gives the analyzer parameter values over a wide range of the operation.



Figure 5. The genetic algorithm solutions for the M versus P₁ and P₂ values for $\alpha=0^{\circ}$, $\Delta r_{\pi}=0$, $\Delta r_{0}=1.97$, D=100 mm.





Figure 6. The genetic algorithm solutions for the M versus Δr_{π} and Δr_0 values for $\alpha=1^{\circ}$, D=100 mm, P₁=P₂=-250.

4. Conclusion

In this study, the base energy resolution of the 180° hemispherical deflector energy analyzers are calculated for optimization over a wide range of parameters. An artificial intelligence method, GA, is used for these calculations. The results have been presented in graphical form to show the effectiveness of the algorithm. The evolutionary computing based GA is useful for experimental studies in terms of giving solutions for many problems with a large number of parameters. While searching for solutions for the base energy resolutions, the fact that being trapped within the local minimums can be prevented by running the GA several times. The results show that the GAs prove to be an efficient tool to provide usable optimal solutions in a short amount of time. The proposed algorithm for HDA base energy resolution equations provides a list of good solutions and not just a single solution. Therefore, the GA method is very useful when the search space is very large and there are a large number of parameters involved. Without using any training dataset like ANN, Regression, etc., the GAs are very simple to apply for many problems and also fast for other methods. This article can guide for experimentalists to acquire optimum parameter values for the HDA having high energy resolution.

Author's Contributions

Murat Ince: Drafted and wrote the manuscript, performed the experiment and result analysis.

Nimet Işık: Assisted in analytical analysis on the structure, supervised the experiment's progress, result interpretation and helped in manuscript preparation.

Ethics

There are no ethical issues after the publication of this manuscript.

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