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Araştırma Makalesi / Research Article

Calculation of Optimum Transit Times with Real-Coded Genetic Algorithm

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Abstract
Electron energy analysers have been designed to analyse charged-particle beams at specific energies. The design is based on the principle that electrons with different energies arrive at the detector at different times. Since electrons with different energies follow different orbits within these analysers. In collision experiments, it is very important to determine the trajectories and transit times of the charged particles in the analyser. In this study, optimum solutions for transit times of charged particles were provided using a real-coded genetic algorithm. Hyper parameters and types of genetic algorithm were obtained using trial and error methods, in this study. The results of this study indicate that genetic algorithm gives time resolution values in a wide data set with high accuracy. The results show that genetic algorithms (GA) are a fascinating approach for solving search and optimization problems.

Keywords: Electron spectroscopy, electron beam, energy analyser, genetic algorithm.

Gerçek Kodlu Genetik Algoritma ile Optimum Geçiş Sürelerinin Hesaplanması

Öz
Elektron enerjisi analizörleri, belirli enerjilerdeki yüklü parçacık ışınlarını analiz etmek için tasarlanmıştır. Tasarım, farklı enerjilerdeki elektronların dedektöre farklı zamanlarda ulaşması prensibine dayanmaktadır. Farklı enerjilere sahip elektronlar bu analizörlerde farklı yörüngeler takip ettiğinden. Çarpışma deneylerinde yüklü parçacıkların analizördeki yörüngelerinin ve geçiş sürelerinin belirlenmesi çok önemlidir. Bu çalışmada, yüklü parçacıkların geçiş süreleri için gerçek kodlu bir genetik algoritma kullanılarak optimum çözümler sağlanmıştır. Bu çalışmada hiper parametreler ve genetik algoritma türleri deneme yanılma yöntemleri kullanılarak elde edilmiştir. Bu çalışmanın sonuçları, genetik algoritmanın geniş bir veri kümesinde zaman çözünürlük değerlerini yüksek doğrulukla verdiğini göstermektedir. Sonuçlar, genetik algoritmaların (GA) arama ve optimizasyon problemlerini çözmek için ilgi çekici bir yaklaşım olduğunu göstermektedir.

Anahtar Kelimeler: Elektron spektroskopisi, elektron demeti, enerji analizörü, genetik algoritma.

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1. Introduction

Hemispherical energy analysers are the most commonly used analysers in electron spectroscopy because of their high energy resolution (Heddle, 2000). In coincidence studies, these instruments have been designed to analyse a charged particle beam at a specific energy (Dogan et. al., 2007; Zouros 2005). Coincidence timing resolution is an important parameter in the design of these analysers (Zouros and Benis, 2005). Electrons reach the detector at different times because electrons with different energies follow different orbits within these analysers. However, the coincidence peak is desired to be a delta function, for coincidence experiments. It was observed that the coincidence peak had a finite width in the experimental results. The predominant reason for this result is the difference in the transit times of electrons that travel different path lengths in energy analysers.

There are several types of electron spectrometers that utilize time for energy separation. In a time of flight spectrometer, electrons are accelerated by an electric field towards a detector. The time it takes for electrons with different energies to reach the detector is used to separate their energies. Electrons with higher energies will reach the detector faster than those with lower energies. Electrons with higher kinetic energy will have higher velocities and thus shorter flight times (Yildirim et. al. 2009). In velocity map imaging electron spectrometers, electrons are first accelerated by an electric field and then pass through a velocity map imaging system (Baguenard et. al. 2004). Velocity map imaging is a technique used to study the velocity distribution of charged particles, including electrons. This system uses a combination of electric and magnetic fields to map the electron velocities onto a detector. The spatial position on the detector corresponds to the electron's velocity, allowing for energy separation based on time-of-flight.

To date, different methods have been applied to improve the energy and time resolution in energy analysers and significant achievements have been recorded (Zouros and Benis, 2005; Imhof et. al.1976; Völkel and Sandner, 1983; Lower and Weigold, 1989; Caprari, 1995; Kugeler et. al, 2003; Shavorskiy et. al., 2014; Sise and Zouros, 2015; Sise and Zouros, 2016). The calculation of resolution parameters directly using well-known methods is generally limited. The resolution parameter values over a wide range are key to determining optimum solution in coincidence studies. Transit time calculations are presented using an approximate model from various publications in the literature (Imhof et. al.1976; Völkel and Sandner, 1983; Lower and Weigold, 1989; Caprari, 1995; Kugeler et. al, 2003; Shavorskiy et. al., 2014). The transit time and energy distributions of electrons using the trajectory simulation software SIMION 8.1 are given by Sise and Zouros (Sise and Zouros, 2015; Sise and Zouros, 2016). Although successful calculations can be found for certain parameters, none are sufficiently flexible to perform well outside its domain.

This study focuses on the use of an artificial intelligence method to obtain time resolution parameters. In recent years, successful applications have been performed to solve problems in atomic and molecular physics and electron optics (Isik, 2015a; Isik 2015b; Isik 2016; Isik and Isik, 2016a; Isik and Isik, 2016b; Isik et. al, 2017; Ince and Isik, 2020). The artificial intelligence method provides exciting alternative calculation method. Genetic algorithm (GA), one of the sub-branches of artificial intelligence is inspired by the process of natural selection (Goldberg, 1988; Goldberg, 1989; Davis, 1991). The GA has proven to be an important research algorithm for solving nonlinear, multivariate optimization problems. GA approaches have been applied to several computational and design problems (Paszkowicz, 2009; Jiang et. al., 2020). The GA is more efficient in solving difficult and discontinuous functions than traditional optimization techniques. Therefore, an important aspect of GA research is function optimization. Because GA is an intuitive method, it may not find the exact result for a given problem, but it provides solutions that are very close to the exact result for problems that cannot be solved by known methods or whose solution time increases exponentially with the size of the problem. GAs generate possible solutions to the problem. In this generation, crossover and mutation processes to create new solutions and reproduction processes to ensure the survival of the best solution are applied to reach a generation with better solutions.

In this study, GA was used for the time-resolution equations of electrons in energy analyzers. This paper is organized as follows: In the Materials and Methods section, the time resolution equations and the GA method are introduced. The next section presents the calculations of transit time distribution in energy analyser using by GA.

2. Materials and Methods

2.1. Time Resolution Parameters

Hemispherical energy analysers are fundamental instruments used in many experimental studies such as high-resolution charged particle spectroscopy and electron-electron coincidence spectroscopy (e,2e). The improvement of these experimental devices requires the optimization of all parameters in the charged particle detection chain, which influence the time resolution. To obtain careful and reliable results in simultaneous multi-particle measurements, the experimental setup must be precisely designed and tested. One of the most important parts of collision spectrometers is the energy analyser which provides an analysis of charged particles.

Hemispherical energy analysers consist of two hemispherical deflectors and an input optics. The input optics focus on the electron beam at the input of the deflectors. Input optics are used to delay the electrons by the voltages supplied to the lenses and to focus the hemisphere input. Pre-retardation is an application that increases the resolution. Therefore, it is very important to know the relationships between the aberration coefficients and magnification parameters in the design of analyser systems. The optimal lens magnification, $|M|$ was calculated as follows:

$$|\mathrm{M}|=\left[\frac{1}{2}\left(\frac{\mathrm{FD}}{\mathrm{d_s}}\right)\left(\frac{\mathrm{d}_\rho}{\mathrm{l}}\right)^2\right]^{1/3} \tag{1}$$

where F is the pre-retardation factor, D is the dispersion, d_s is the incident beam spot and is given by the formula $d_s = \Delta r_0/M$, and Δr_0 is the diameter of the aperture at R_0, d_ρ is the diameter of lens entrance aperture. The pre-retardation factor, F is related to the entry bias V_0. This relationship is given by the following formula:

$$\mathrm{qV_0}=(\mathrm{F}-\gamma)\mathrm{E_0} \tag{2}$$

The electrons are distinguished according to their energy and reach the detector because of the voltages applied to the inner and outer deflectors. As shown in Fig. 1, electrons enter the deflectors at a small value of α. Electrons are focused on the analyser input with the help of the input optics. They follow an elliptical trajectory in the electrostatic field of hemispherical electrodes according to their energies.

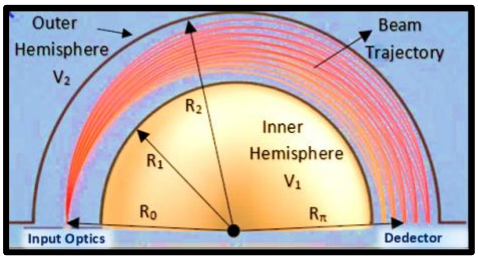

Figure 1. A section through the hemispheres of the HDA. R_0 is circular path radius of charged particle beam in the hemispheres. R_1 and R_2 are the radii of the two concentric inner and outer hemispheres, respectively. V_1 and V_2 stands for the voltages of the inner and outer hemispheres, respectively. In an ideal HDA, an electron with charge q and energy E enters the deflector area through the aperture of diameter Δr_0 with an angle α. The electron exits in r_π after following an elliptical orbit. The central trajectory is defined by a particle that enters the deflector field at $r_0 = R_0$ and exits the deflectors at $r_\pi = R_\pi$.

However, the charged particle beam that follows different trajectories reaches the detector at different times. The differences in the times required to reach the detector affect the time resolution. Within the hemispheres, the transit times of the charged particles, t_π is given by formula (Caprari, 1995),

$$t_{\pi}=\frac{T_0}{2\pi}\left\{\pi+2\arctan\left[\sin\alpha\sqrt{\left(-1+\frac{2}{\rho_0}\right)}\right]-\frac{4\left(\sqrt{\frac{\rho_0}{2-\rho_0}}\right)\sin\alpha}{\cos2\alpha-\left(\frac{2+\rho_0}{2-\rho_0}\right)}\right\} \quad (3)$$

where T_0 stands for the period of the Kepler orbit, which is calculated from $T_0=2\pi(ma^3/qk)^{1/2}$, α is the angle of the electrons entering the analyzer, $\rho_0=r_0/a$ where r_0 is the mean beam radius. a is given by the formula $a=-q\left(\frac{R_1R_2(V_2-V_1)}{R_2-R_1}\right)/2E$. R_1 and R_2 are the radii of the concentric inner and outer hemispheres, respectively. V_1 and V_2 represent the voltages of the inner and outer hemispheres, respectively.

2.2. Genetic Algorithm

Knowledge of the difficulty level of the problem enables the application of the best method for solving the problem. Polynomial algorithms perform well when solving practical problems. The polynomial algorithms used in non-polynomial (NP) bounded problems cannot solve the problem. In the solution of NP problems, close solutions are preferred over exact results. Because the exact results of such problems cannot be reached in a short time, approximate solutions are obtained by local and random searches. The GA is a research method that attempt to find a solution using random search techniques. It is an algorithm that attempt to find the most suitable (best for purpose) among the many possible solutions to a problem. The GA is used in cases where there are many factors that affect the problem. In this study, GA was used because the transit time problem of electrostatic lenses is a multicriteria problem.

One of the basic components of the genetic algorithm is a gene. Genes are encoded representations of the optimization parameters of each problem. Chromosomes are formed by arranging genes in a certain order using a genetic algorithm. Chromosomes are alternative solution. Chromosomes can be encoded differently depending on the problem. The first step in the implementation of GA is to choose the coding structure that best represents the problem. In this study, a real-coded GA was selected to represent the problem. A population is a valid set of alternative solutions. It can be defined as the set of chromosomes used by the genetic algorithm uses to search for the most suitable solution. In the flowchart shown in Fig. 2, these steps are applied to the generated chromosomes. This process repeats until the stopping criterion is satisfied.

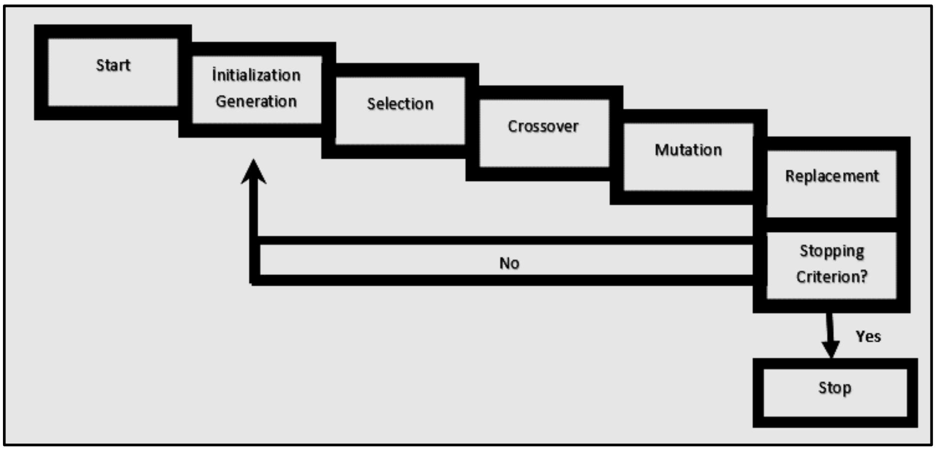

Figure 2: The flowchart of the GA.

The selection mechanism used in this study was roulette wheel selection. In this selection, the circle was divided into n particles. Each range represented a sequence. The fitness value of each sequence was divided by the total fitness value. Thus, each array has its own place among its values in the solution set. For reproduction, a random number between zero and the total fitness is generated and the chromosome is selected by looking at which part of the wheel this number falls on. Similarly, all the chromosomes were identified. The most successful individuals with fitness values are taken into the matching pool and a new generation was obtained.

As there is no generational diversity after certain points when examining the solution stack, a solution cannot be reached. To achieve this, generation diversity is provided by applying cross over and mutation operators to the sequences. Thus, the system is prevented from reaching certain points and getting stuck. Crossover is the displacement of specified parts between two individuals. A very low replacement probability may result in the loss of some features. This hinders the determination of an optimal solution. However, a high probability of replacement may degrade the existing solutions. In this study, a uniform crossover operator with a crossover probability of 0.75 was chosen to ensure gene diversity. In the next step, a multi-point mutation operator with a mutation rate of 0.01 was applied to scan the research space without the problem of early convergence. The search for the roots of the equation continued until 1000 iterations or the exact value of the function value was less than $E=10^{-5}$.

3. Findings and Discussion

In this study, GA was used to find the minimum transit time (t_π) as a function of the conserved total energy of electrons (E) using Eq. (3). The specific spectrometer parameters were used in the present calculation: R_0=82,55 mm, R_1=72,40 mm, R_2=130,80 mm, γ=1,50; d_s=2,50 mm, $d\rho$=4,00 mm, l= 288,50 mm. The fitness function to be minimized for transit times can be obtained using Eq. 3 where the boundaries for the angular spread of the electrons are $0° \leq \alpha_0 \leq 3°$. The first step in GA coding is to select the coding structure that best represents the search space for a problem. Real-coded GA is used in this study. In the next step, the initial population is generated. Population size is 100. Each chromosome was evaluated according to the fitness function. The best fit chromosomes were selected. The selected chromosomes were then reproduced by crossing over and mutating. This process was repeated until the stopping criterion was satisfied. Fig. 3a shows the GA optimum solutions for the time distributions at the exit of the HDA. A representation of the GA approximate solutions obtained by the search is shown in Fig. 3b. Fig. 4 shows pre-retardation values as a function of aperture diameter at the entrance to the deflectors.

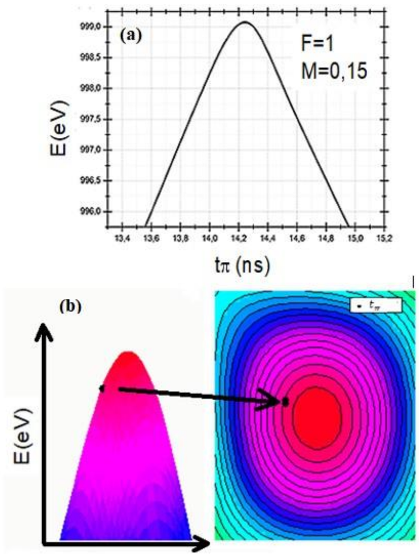

Figure 3. (a) The transit times of the charged particles, t_π as a function of their energies**,** E. **(b)** Optimum solutions for the transit times of the charged particles, t_π provided by genetic algorithm search.

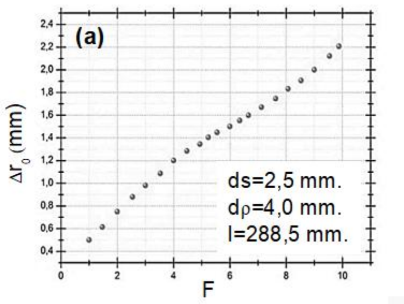

Figure 4: The values of the virtual entry aperture size as a function of the pre-retardation ratio F.

One of the most significant factors determining the performance of the proposed GA is population diversity. The average distance between individuals at each generation is one of the most important factors affecting the performance of GAs. Fig. 5 shows the average distance between individuals at each generation for the time-resolution problem. The graph showing the suitability of the best solution for the problem of transit times either decreases compared to the previous iteration or remains at the same level until better solutions are found. Fig. 5 presents a critical analysis of the performance of the proposed Genetic Algorithm (GA) in terms of population diversity for the time-resolution problem. Population diversity is a crucial factor influencing the effectiveness of GAs, as it determines the exploration capability of the algorithm across the solution space. The average distance between individuals at each generation serves as a metric to measure this diversity. The graph in Fig. 5 illustrates the trends in the average distance between individuals over successive generations. A higher average distance between individuals indicates greater diversity, implying that the GA is effectively exploring different regions of the solution space. This diverse exploration is essential for avoiding premature convergence and finding better solutions. Furthermore, Fig. 5 also presents a plot depicting the suitability of the best solution found by the GA for the transit times problem. In an efficient GA, this suitability should ideally improve over iterations as better solutions are discovered. However, the graph suggests that in certain cases, the suitability of the best solution may either decrease compared to the previous iteration or remain stagnant until better solutions are found in subsequent generations. The observed fluctuations in the suitability of the best solution can be attributed to the inherent stochastic nature of GAs. During certain iterations, the algorithm may encounter less favorable regions of the solution space, leading to a temporary decrease or stagnation in solution quality. However, as the GA continues its search and maintains population diversity, it is likely to discover more promising regions, leading to improved solutions in the long run.

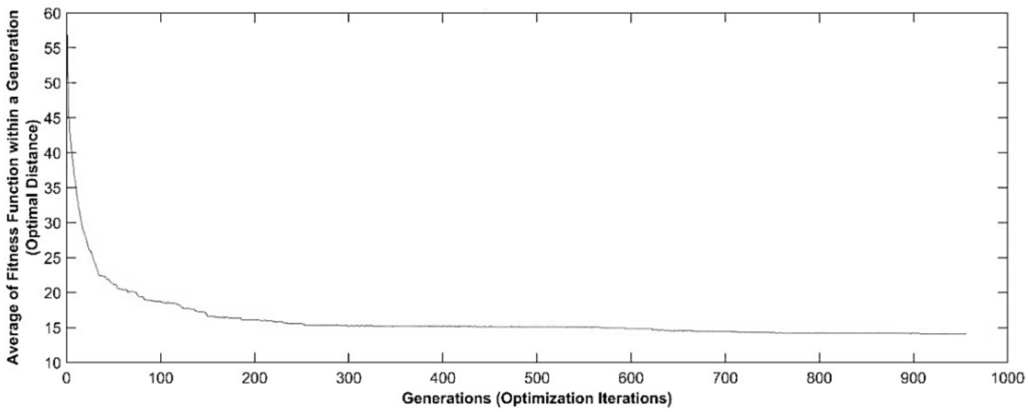

Figure 5: Optimal distance of all individuals in each generation for transit time calculation.

4. Conclusions and Recommendations

Transit time distribution of electrons is characterized by the concept of time resolution. The time resolution depends on many parameters such as the angle and energy of the electron beam. In this study, transit time distributions were determined using the genetic algorithm (GA) method. A genetic algorithm is a research method that attempts to find a solution in a group by using random search techniques and thus chooses the best solution among many solutions. In this study, the best solution hyper parameters were determined to be uniform crossover with a rate of 0.75 and mutation rate of 0.01. The results of this study indicate that genetic algorithm gives the time resolution values in a wide data set with high accuracy. The results show that genetic algorithms (GA) are a fascinating approach for solving search and optimization problems. Hyper parameters and types of genetic algorithm were obtained using trial and error methods, in this study. This algorithm makes it possible to determine the time resolution parameter significantly more accurately and efficiently than the approximate methods.

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Statement of Conflicts of Interest

There is no conflict of interest between the authors.

Statement of Research and Publication Ethics

The author declares that this study complies with Research and Publication Ethics. This study was presented at the 2nd International Symposium on Characterization.

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