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Time Series Artificial Neural Network Approach for Prediction of Optical Lens Properties

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Well-designed electrostatic cylindrical lenses are commonly used to control charged particles in atomic and molecular physics instruments such as electron guns and electron microscopes. The most commonly used of these, three-element electrostatic lenses are capable of keeping magnification constant for definite image position. The correct determination of focal and aberration characteristics of these lenses is very important for experimental studies. In this study, motions of electrons in three-element electrostatic cylindrical lenses have been investigated with nonlinear autoregressive exogenous based time series artificial neural network technique. The spherical and chromatic aberrations which affect the beam are also predicted with time series artificial neural network technique. This method is a mathematical model that emulates the biological neural networks. The basic working principle of time series artificial neural network technique is training of network with the known data and then prediction of the unknown data. Simulation results from SIMION 8.1 ray-tracing program are used as training and test data set. According to the results obtained from time series artificial neural network technique technique, a considerably agreement is found between simulation and artificial neural network technique prediction results. The study shows that such an artificial neural network model which has time advantage can be applicable to various electron and ion beam apparatus.

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1. Introduction

Electron optical systems are widely used in many scientific instruments, such as electron microscopes, time of flight spectrometers, and electron guns [1, 2]. Among these optical tools, three-element electrostatic cylindrical lens systems are perfectly suited to use in collision experiments [3, 4]. These lenses can be effectively operated with different magnifications while keeping the image points. Although the investigations of optical properties for such a lens have a long tradition, the optical properties are still studied with different techniques [5–7]. New milestone method for modeling problems in optical physics is artificial intelligence application [8, 9]. Pilot studies demonstrating the capabilities of the artificial neural networks have predicted optical parameters with tremendous precision [10]. Our goal is the establishment of artificial neural network approach to solve the imaging properties with aberration coefficients for three-element cylindrical electrostatic lenses. Obtained results show that artificial neural networks have learned the complex relationship between the lens voltages and electron beam size in definite image position. In comparison with the proposed methods in literature, time-series artificial neural network (TSANN) method is advantageous for rapid prediction.

This study is organized in four sections. In Sect. 1, introductory information regarding the electron optical systems and artificial neural network are given. In Sect. 2, detailed information about three-element cylindrical lenses and TSANN are given briefly. The results and discussions are given in Sect. 3. Finally, conclusions regarding analysis of optical lens properties with the spherical and chromatic aberrations through are given.

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2. Method

In experimental collision studies, three-element cylindrical lenses have been generally used to obtain focused electron beam in definite position. In Fig. 1, the distribution of electron beam dependence on the radial displacement is obtained by plotting the trajectories of electrons. The launching angles are varied between 0° and ±5°. The optimal focus point is obtained in image point (Fig. 1c).

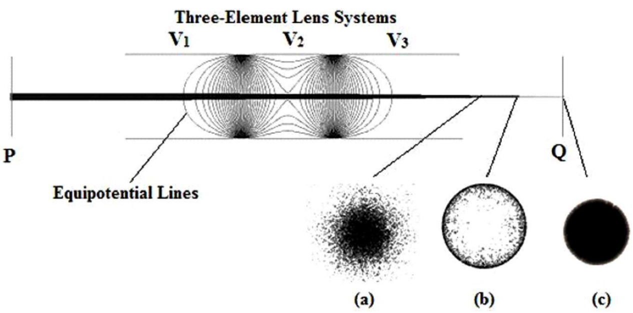

Fig. 1. Observing the focusing of electrons in the XY plane using the three-element lens system: (a) non-focused condition, (b) electron distribution close to the focus region, (c) focused condition.

This focusing situation provided with the applied voltages of lens elements are mostly affected with the spherical and chromatic aberration coefficients. Electrons which are entered to the lens systems with different angles are focused in different image points. This is known as a spherical aberration. The spherical aberration coefficient (C_s) is defined by the following formula:

$$\Delta r = -MC_s\alpha_0^3, \quad (1)$$

where Δr is the radius of the disc in image point, M is the linear magnification, and α_0 is the maximum half angle for electrons entering from a given object distance (P). The electrons with different energies are also focused at different image planes. This deflection is defined by the chromatic aberration coefficients for a lens system. The relationships between the energies of electrons and chromatic aberration coefficient (C_c) is defined by the following equation where δr is the spread in image distance [5]:

$$\delta r = -MC_c\alpha_0\frac{\delta V}{V_0}. \quad (2)$$

It is well known that these aberrations can be minimized by correct electrostatic lens voltages in experimental lens designs. In this study, the nonlinear autoregressive exogenous (NARX) based TSANN technique is applied to the optical properties of three-element lenses taking into account the spherical and chromatic aberrations. The TSANN is a kind of recurrent network and has an ability to solve complex problems. It is based on the fact that the TSANN learns the relationship between input and output data inspired by human brain. With this feature, it predicts the unknown data by using previously given data. In programming of simulation, input and output values are converted to the sequential vectors and lens dataset is randomly divided into the three groups. Tapped delay line is also used for both inputs and outputs. Then, NARX network is constructed and input and output time series data for network simulation is prepared. After that, training and simulation are performed.

3. Results and discussion

In this study, the electron optical properties of a three-cylinder electrostatic lenses configuration are investigated by means of NARX based TSANN method. These lens system consists of three-cylinders of the same diameter D (= 100 mm). All parameters are quoted to the lens diameter such as P/D and Q/D. Figure 2a shows the relationship between V_2/V_1 and V_3/V_1 for a constant object ($P/D = -5$) and image point ($Q/D = 5$). The dependence of the magnification values on V_3/V_1 are shown in Fig. 2b. It is clear that the ANN prediction data for voltage ratios and magnification are consistent with the SIMION simulation data with the error in the range of 0.1–0.3%. In this study, the training data set consists of 96 input data of voltage ratios and the 96 output data set of magnification and aberration coefficient values.

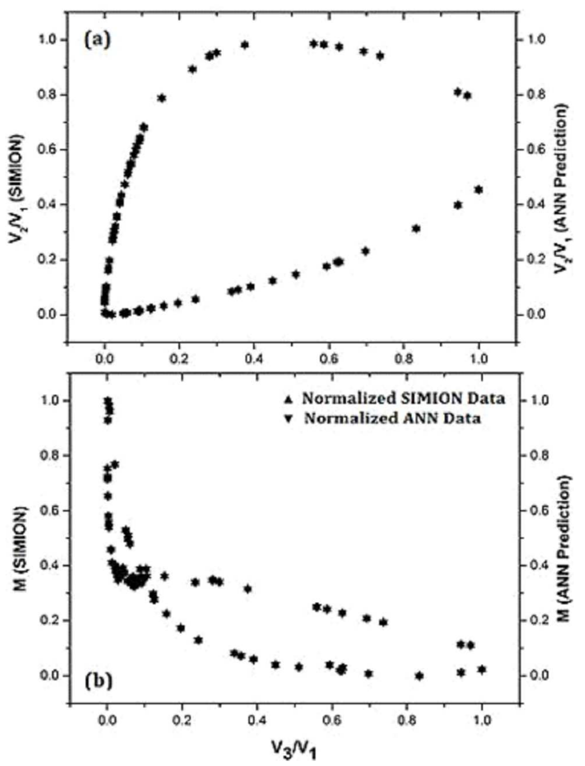

Fig. 2. The relationship between V_2/V_1 and V_3/V_1 and magnification values (M) as a function of V_3/V_1 for three-element cylinder electrostatic lens system. ▲: SIMION data. ▼: ANN prediction data. Note that the values are normalized to range of [0, 1].

In Fig. 3a and b, the spherical (C_s) and chromatic aberration coefficients (C_c) obtained by TSANN method are shown, respectively. For comparison, the SIMION simulation data are given in the same figures. As can be seen in Fig. 3a and b, the prediction data of TSANN method are found to be a good agreement with the SIMION simulation data. This predictive power of TSANN is performed with the training an optimum input/output pairs.

In the proposed TSANN, number of hidden layers is determined with the optimum compliance with the SIMION simulation input data set. The network is trained using the Levenberg–Marquardt optimization technique [11]. Using the input/output values, different network configurations were trained to obtain minimum mean squared error (MSE) and maximum regression values. In present study, the network architectures for NARX based TSANN model is given in Table I. Among these architectures, 2-24-3 provides best prediction results for focal and aberration characteristics of lenses. This architecture has 1, 0.984, and 0.999 regression values for training, validation, and testing respectively. MSE value is obtained as 1.63×10^{-24}.

One regression result means close relationship between variables, conversely, zero means weak relationship. Training result of 2-24-3 network has one regression value and it is given in Fig. 4. In addition, test result shows that TSANN predicted unknown data perfectly.

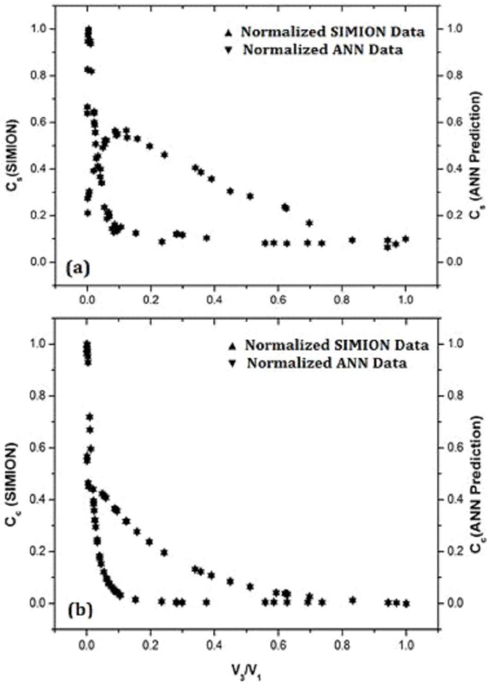

Fig. 3. The relationship between spherical (C_s) and chromatic aberration coefficients (C_c) as a function of V_3/V_1 for three-element cylindrical electrostatic lens system. ▲: SIMION data. ▼: ANN prediction data. Note that the values are normalized to range of [0, 1].

TABLE I

Regression, MSE and epoch results for different architecture.

Architecture	Regression			MSE	Epoch
	Training	Validation	Test		
2-10-3	0.955	0.888	0.922	0.022	1000
2-12-3	0.986	0.896	0.940	0.007	1000
2-14-3	0.990	0.946	0.964	0.005	1000
2-16-3	0.994	0.955	0.966	0.003	1000
2-18-3	0.999	0.966	0.954	0.002	1000
2-20-3	0.999	0.968	0.978	0.001	502
2-22-3	1	0.972	0.996	9.86×10^{-10}	138
2-24-3	1	0.984	0.999	1.63×10^{-24}	78
2-26-3	1	0.982	0.999	4.21×10^{-21}	130

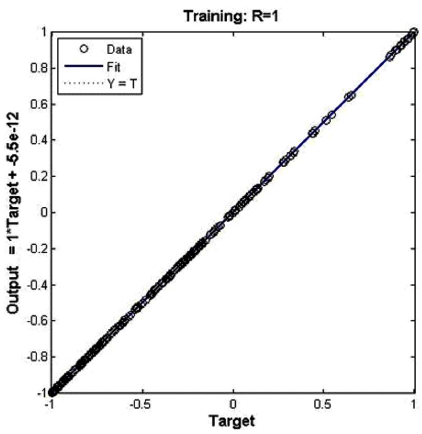

Fig. 4. Regression results of training.

4. Conclusion

Main purpose of the study is to investigate the usefulness of artificial neural network in optical lens systems. In this context, NARX based TSANN is used to predict the magnification and aberration coefficients for three-element electrostatic cylindrical lens. We found high performance results through regression and MSE values. The results show that TSANN can be used to predict unknown data for optical lens systems. This approach is an alternative and powerful technique for this field. In the future, we will validate the performance of the TSANN using experimental values instead of simulation data. Moreover, different prediction technique can be used for this dataset.

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