



## Original Article

## Neuro-fuzzy modeling of deformation parameters for fusion-barriers

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## ABSTRACT

The fusion-barrier distribution is very sensitive to the structure of the colliding nuclei such as nuclear quadrupole and hexadecapole deformation parameters and their signs. If the nuclei that enter the fusion reaction are deformed, the barrier problem becomes complicated. Therefore the deformation parameters are taken into account in the calculations. In this study, Neuro-Fuzzy approach, ANFIS, method has been used for the estimation of ground-state quadrupole ( $\epsilon_2$ ) and hexadecapole ( $\epsilon_4$ ) deformation parameters for the nuclei. According to the results, the method is suitable for this task and one can confidently use it to obtain the data that is not available in the literature.

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## 1. Introduction

In the fusion process [1], a compound nucleus is formed after overcoming a fusion barrier created between nuclei from repulsive Coulomb and attractive nuclear forces. The fusion barrier distribution [2] which is important for the understanding of fusion mechanism is sensitive to the data related to some nuclear properties such as the nuclear shapes, deformations, multiple excitations and the nuclear surface vibrations [3]. This distribution not only depends on the static quadrupole deformation but also on the hexadecapole deformation [4]. Furthermore, the fusion cross-section depends on the ground-state shapes of the nuclei related to the deformation parameters [5]. Fusion cross-sections have been increased in energies around the Coulomb barrier compared to the estimation of a simple potential model as a result of Coulomb barrier distribution depending on the deformed target nucleus orientation [6,7]. By using spherical projectile and target nuclei, the fusion-barrier penetration problem is easy whereas if the nuclei are deformed, the problem becomes complex [8]. For the detailed information about the effect of the shapes on the fusion-barrier distributions and the fusion-cross section, we refer the reader to Iwamoto [9].

Since fusion is an absorption process from the coupled-channel system, the coupled-channel model calculation [10], one of the common theoretical models for the task, permits to obtain accurately the fusion cross-section for the not very heavy target and projectile nuclei [11]. These calculations have to account for the nuclear deformations of the projectile/target and the associated fusion barrier distribution [9]. The deformation parameters are obtained either from experimental data or calculated theoretically from nuclear masses and ground state shapes [12]. The  $\epsilon$  parameterization for the deformations was used originally in the Nilsson modified-oscillator model [13]. These are used in many fields to investigate several nuclear phenomena. For instance, the ground-state potential energy is calculated as a function of  $\epsilon_2$  and  $\epsilon_4$  parameters and the minimum are identified. It was introduced to simplify the calculation of matrix elements between nuclear single-particle wave functions. The  $\epsilon_i$  parameters are highly related to the fusion barrier height. A large, positive value of the hexadecapole deformation parameter yields a lower fusion barrier [14].

Artificial intelligence approaches have been used in many fields in nuclear physics studies. The following studies can be given as examples of the studies performed by our group. Determination of ground-state energies of the nuclei [15], estimations of beta decay energies through the nuclidic chart [16], estimations of fission barrier heights [17], estimations of fusion reaction cross-sections [18]. Artificial intelligence tools provide shorter development processes, good approximation capabilities and fast processing time. Fuzzy logic which one of the common artificial intelligence tools

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has been regarded as a conventional tool [19]. Fuzzy inference system based modeling is very successful in solving real-world problems such as approximation of a function, time series forecasting, controlling dynamic systems and solving differential equations, etc. [20] Adaptive Neuro-Fuzzy Inference System (ANFIS)

$$\begin{aligned}
 R_1 : \text{if } Z \text{ is } A_1 \text{ AND } N \text{ is } B_1 \text{ AND } A \text{ is } C_1 \text{ then } f_1 &= p_1Z + q_1N + r_1A \\
 R_2 : \text{if } Z \text{ is } A_2 \text{ AND } N \text{ is } B_2 \text{ AND } A \text{ is } C_2 \text{ then } f_2 &= p_2Z + q_2N + r_2A \\
 \dots & \dots \\
 R_k : \text{if } Z \text{ is } A_k \text{ AND } N \text{ is } B_k \text{ AND } A \text{ is } C_k \text{ then } f_k &= p_kZ + q_kN + r_kA
 \end{aligned} \tag{1}$$

that combines the fuzzy inference system and training capability of the neural network is one of the most common fuzzy tools for nonlinear function approximation and input-output modeling [21]. Particularly, ANFIS method has also been used in fusion studies such as prediction of neutron yield of inertial electrostatic confinement fusion device [22], forecasting the error in EAST Articulated Maintenance Arm working in tokamak fusion reactor [23], joints controlling steam generator water levels in nuclear power plants [24], the evolution of a neutron energy spectrum unfolding code [25], prediction of the nuclear tracks [26], determination of the fragility curves in degraded nuclear power plant [27] and determination of boron concentration in a pressurized water reactor [28]. Best of knowledge, although there are many real-world applications of neuro-fuzzy approaches, there is no research work focuses on the estimation of deformation parameters for the nuclei. In this study, ANFIS method has been used for the estimation of ground-state quadrupole ( $\epsilon_2$ ) and hexadecapole ( $\epsilon_4$ ) deformation parameters for the nuclei. The data have been borrowed from Möller et al. [29] including 1182 data points from atomic number 8 to 108. In this reference, deformation parameters have been classified into two separate groups according to the axial and reflection asymmetries since the axial and reflection-asymmetric shape degrees of freedom affect the ground-state nuclear mass.

## 2. Material and methods

### 2.1. Adaptive neuro-fuzzy inference system for deformation parameter estimations

Fuzzy set concepts were proposed by Zadeh as an extension of the crisp set theory [30]. A fuzzy set provides an element  $x$  has a degree of membership instead of being 0 or 1. Fuzzy inference provides set operation for fuzzy sets. Fuzzy inference system and Fuzzy controller has been widely used in many real-world problems for past decades. ANFIS is a hybrid approach that combines a fuzzy inference system and neural network. Fuzzy inference system is a good representative of the knowledge system with if-then rule base while it needs expert knowledge to tune the number of rules, membership functions. The neural network is capable of tuning its synaptic weight with error back-propagation if data were available. Therefore, the hybridization of a fuzzy inference system with neural networks brings into the learning capability of a fuzzy inference system.

There are two main approaches for the fuzzy inference system as Mamdani and Takagi-Sugeno types [31]. Although both approaches use fuzzy sets for input, Takagi-Sugeno uses a linear function of inputs for output [21]. The rule base of the fuzzy inference system can be constructed with a heuristic approach or expert knowledge if there was prior information between input

and output for the Mamdani type approach [19]. In the lack of prior information or expert knowledge about input-output relation, the Takagi-Sugeno approach provides the construct the rule base by clustering the input-output data [31]. Rule base system for the current problem with Takagi-Sugeno type Fuzzy inference system

is given as bellows as

where  $A_{1,2,\dots,k}$ ,  $B_{1,2,\dots,k}$  and  $C_{1,2,\dots,k}$  fuzzy sets for input  $Z$ ,  $N$  and  $A$  respectively for total  $k$  rule.  $f$  is an output function which is a linear combination of inputs. For each instant, each input corresponds to a degree of membership concerning the belonging fuzzy set. In this work, it is used Gaussian type membership function for each fuzzy set to calculate the degree of membership as;

$$\mu_{A_j}(Z) = e^{-\frac{1}{2} \left( \frac{z - c_j^k}{\sigma_j^k} \right)^2} \tag{2}$$

$$\mu_{B_j}(N) = e^{-\frac{1}{2} \left( \frac{n - c_j^k}{\sigma_j^k} \right)^2} \tag{3}$$

$$\mu_{C_j}(A) = e^{-\frac{1}{2} \left( \frac{a - c_j^k}{\sigma_j^k} \right)^2} \tag{4}$$

where  $\mu_{A_j}(Z)$ ,  $\mu_{B_j}(N)$  and  $\mu_{C_j}(A)$  are the degree of for  $j$ th rule membership for crisp inputs  $Z$ ,  $N$  and  $A$  respectively.  $c_j^k$  and  $\sigma_j^k$  correspond center and spread of gauss membership function. Hybridization of a fuzzy inference system with neural network mainly focuses on training parameters of fuzzy inference system with back-propagation of error signal. The general framework of ANFIS proposed by Jang with Takagi-Sugeno fuzzy inference system was modified for the current approach was shown in Fig. 1.

ANFIS architecture consists of 5 layer networks as given below.

Layer 1: Fuzzify the crisp inputs to fuzzy value with the degree of membership value as described in Eqs. (2)–(4).

Layer 2: Calculation of each rule firing strengths as

$$w_j = \mu_{A_j}(z) \cdot \text{AND} \cdot \mu_{B_j}(n) \cdot \text{AND} \cdot \mu_{C_j}(a) \tag{5}$$

where fuzzy AND operator is used as either minimum operation or product operation.

Layer 3: Normalize each firing strength concerning the sum of all firing strengths as

$$w'_j = \frac{W_j}{\sum_{l=1}^k W_l} \tag{6}$$

Layer 4: Defuzzify the fuzzy value to crisp value by defuzzification

$$w'_j f_j = w'_j (p_j z + q_j n + r_j a) \tag{7}$$

Layer 5: Calculate the overall output

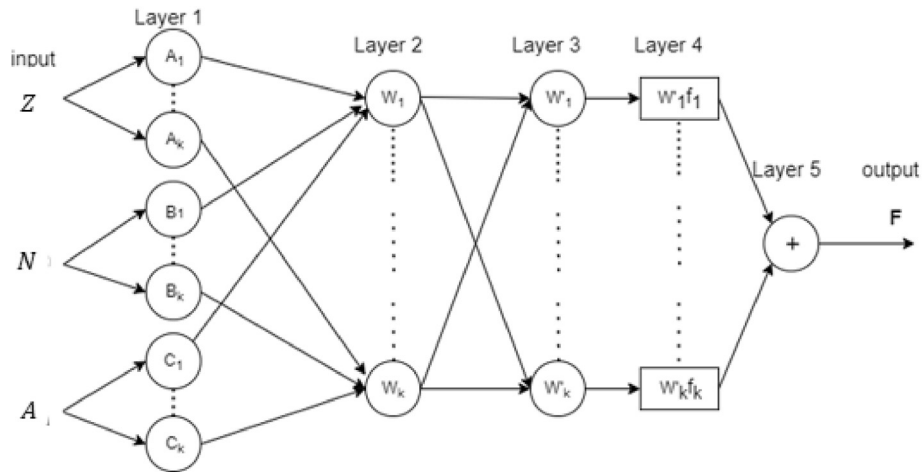


Fig. 1. Adaptive neuro-fuzzy inference system for deformation parameter estimations.

$$F = \sum_{j=1}^k w'_j f_j = \frac{\sum_{j=1}^k w_j f_j}{\sum_{j=1}^k w_j} \tag{8}$$

$$RMSE = \left[ \frac{1}{n} \sum_{i=1}^n |f_i - \hat{f}_i|^2 \right]^{\frac{1}{2}} \tag{10}$$

Initial membership function parameters and the number of membership could be initialized with the clustering algorithm as subtractive clustering or fuzzy C-means clustering [31]. Least square estimation could tune linear parameters in rule consequent parts as described in Eq. (1) for Sugeno type Fuzzy inference system. Nonlinear parameters in rule antecedent part could be tuned by gradient descent based error back-propagation methods.

### 2.2. Experimental setups

All codes are developed as Matlab (Matlab R2018b) function with an intel i7 desktop computer. Data are portioned as training, validation and test parts with a 5-fold validation procedure. Therefore, ANFIS has been trained, validated and tested with different data set for each 5 fold. Initial fuzzy sets and fuzzy if-then rule bases were constructed with subtractive clustering methods. Clustering radiuses were chosen for subtractive clustering as 0.1 for input *Z*, *N* and *A*. It yields the number of clusters that corresponding to the number of the if-then rule as 40 and 45 for estimation of quadrupole ( $\epsilon_2$ ) and hexadecapole ( $\epsilon_4$ ) deformation parameters respectively. Linear parameters in the rule consequent parts were trained by the LSE method while parameters of membership function were trained by error back-propagation method. Epoch number for gradient descent based training was set to 250. Membership function type was chosen as the Gaussian membership function for all input variables. Fuzzy AND operator was selected as a product operator that produces rule firing strength by product of each degree of membership values. The implication method was also selected as Fuzzy product operation for rule implication.

In order to assess the estimation performance of ANFIS based deformation parameter, two error performance indexes were used. Mean absolute error (MAE) was calculated by

$$MAE = \frac{1}{n} \sum_{i=1}^n |f_i - \hat{f}_i| \tag{9}$$

Root mean square error (RMSE) was calculated by

where  $f_i$  is the actual value,  $\hat{f}_i$  is the predicted value for  $n$  instants. To assess modeling performance of estimation quadrupole ( $\epsilon_2$ ) and hexadecapole ( $\epsilon_4$ ) deformation parameters for the atomic nuclei both training and test phase performance were examined with different test and training data. Therefore, a 5-fold cross-

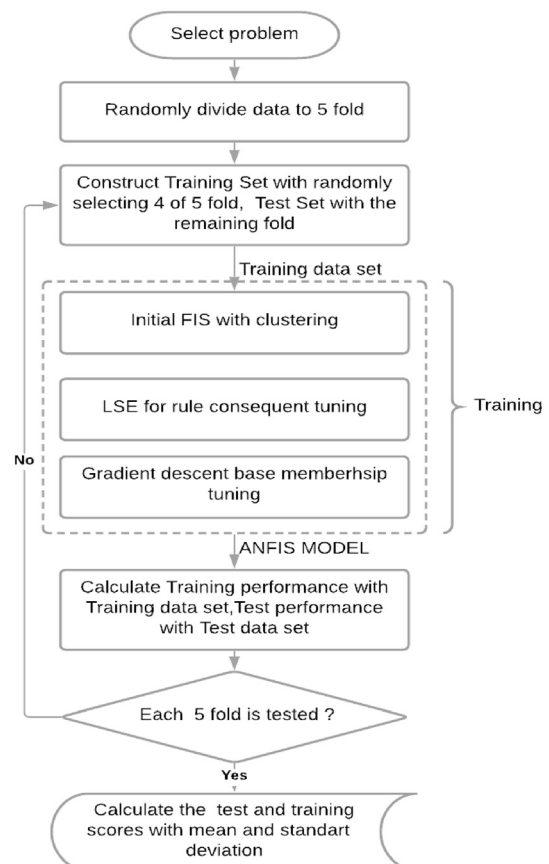


Fig. 2. Flow chart of the model training and evaluation.

validation technique that selects data randomly for each 5 fold is applied to data to portions as 80% for training and % 20 for testing. The flow chart of the training and evaluation of the model is shown in Fig. 2. The algorithm starts with selecting the estimation problem as either  $\varepsilon_2$  or  $\varepsilon_4$ , then 5-fold cross validation operation is performed to obtain training and test set. Initial FIS structure is constructed with clustering the training data. The linear coefficients for rule consequents of the constructed FIS structure, is tuned with LSE method. Finally, parameters of membership function of the rule antecedent part are tuned with Gradient Descent to form trained ANFIS model. Training score is calculated for each iteration with 4 of the 5 fold while test score is calculated with performing the remaining 1 fold data which has not been used in training phase. The model is trained and tested for 5 times with changing the training and test set according to 5-fold cross-validation.

### 3. Results and discussions

In this study, to obtain quadrupole ( $\varepsilon_2$ ) and hexadecapole ( $\varepsilon_4$ ) deformation parameters for the atomic nuclei. ANFIS method has been applied to the literature data borrowed from Möller et al. [14]. In the calculations, both  $\varepsilon_2$  and  $\varepsilon_4$  data have been used separately for axial asymmetry and reflection asymmetry. But  $\varepsilon_2$  ( $\varepsilon_4$ ) values belonging to the two different asymmetries were plotted in the same graphs since they are the same indicator for the deformations.

In the first part of the study,  $\varepsilon_2$  estimations have been performed. The fact that the training error value for ANFIS given in Fig. 3 a reaches about  $7.7 \times 10^{-3}$  indicates that the method is quite reliable.

We have shown in Table 1 that the RMSE and MAE values between actual literature data and ANFIS outputs on both training and test data sets for  $\varepsilon_2$ . The average value of  $\varepsilon_2$  is 0.1663 for all nuclei. As can be seen in the table that the mean RMSE values of a total of 5 folds are in the range of 0.0118 and 0.0415 for training and test data sets. The minimum RMSE has been achieved in fold numbers 3 and 5 for training data and folds number 4 for test data. The mean MAE values are 0.0075 and 0.0188 for training and test data sets. In fold numbers 5 and 3 for training and test data set, respectively, minimum values for MAE have been obtained. We have also given the standard deviations (StD) of the folds in the same table. The small StD proves the model is reliable by showing that RMSE and MAE do not vary much even though the data changes in each fold.

**Table 1**

The calculated performance indices for estimation  $\varepsilon_2$  in the training and test phase in each fold.

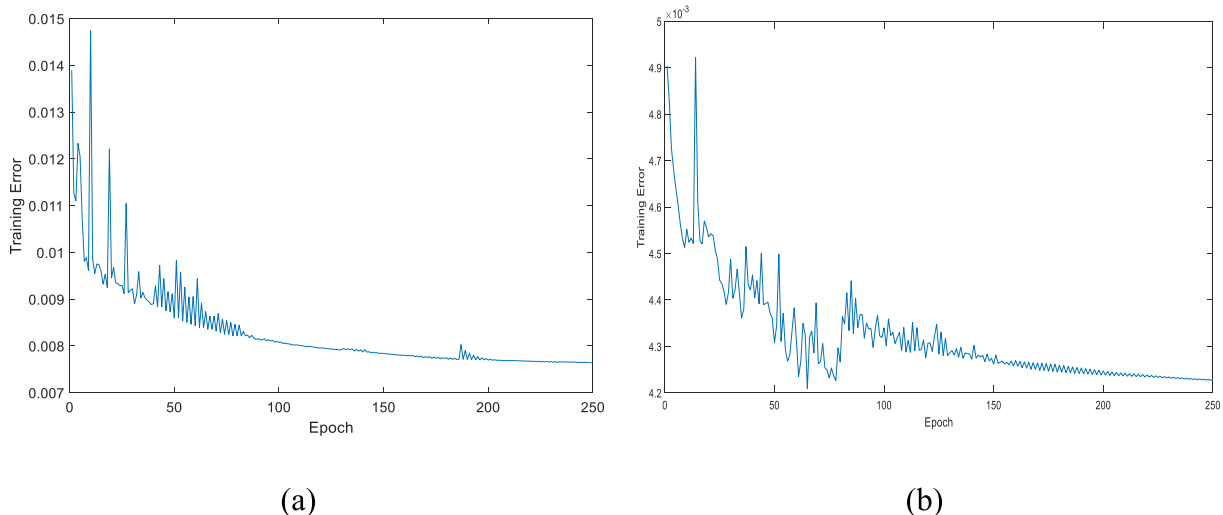
$\varepsilon_2$	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	Mean	StD
Test RMSE	0.0723	0.0305	0.0308	0.0216	0.0525	0.0415	0.0206
Train RMSE	0.0115	0.0124	0.0107	0.0139	0.0107	0.0118	0.0014
Test MAE	0.0220	0.0189	0.0173	0.0145	0.0214	0.0188	0.0031
Train MAE	0.0080	0.0079	0.0073	0.0077	0.0064	0.0075	0.0007

In Fig. 4, we have shown the performance of the methods on the training and test data sets by the estimation of the  $\varepsilon_2$  values. The figure belongs to the fold numbers which gives the best results. The comparisons between actual data and the ANFIS outputs have been done together with the corresponding error values. As is clear in figures that the ANFIS outputs are highly compatible with the non-linear literature data. The differences between literature data and ANFIS output are concentrated around the 0 line by getting maxima as about 0.05 and 0.1 for training and test data sets, respectively. In Fig. 5 a, we have also given the newly generated  $\varepsilon_2$  values for the nuclei. As can be seen in the figure that the quadrupole deformation parameters are mostly positive and get the maximum values of 0.35 in the region of  $Z = 95-98$  and  $N = 129-131$ .

In the second part of the study,  $\varepsilon_4$  estimations have been performed. The fact that the error value in the training of the network is about  $4.2 \times 10^{-3}$  after 250 epochs that indicates that the method is convenient for this task (Fig. 3b).

In Table 2 we have given the related errors according to the different folds on both training and test data sets for  $\varepsilon_4$ . The average value of  $\varepsilon_4$  is 0.0313 for all nuclei. As can be seen in the table that the mean RMSE values of a total of 5 folds are 0.0041 and 0.0100 for training and test data sets. For the estimation of  $\varepsilon_4$  values, the minimum RMSE has been achieved in fold number 3 for training data and fold number 1 for test data. The mean MAE values are 0.0027 and 0.0060 for training and test data sets. In fold numbers 4 and 1, the minimum values have been obtained for training and test data set, respectively. The StD values according to the folds have also been given with the mean and standard deviation values in the table.

We have shown the ANFIS results in comparison with the available literature data of  $\varepsilon_4$  (Fig. 6). We have represented the figures belonging to the fold numbers of the best results. The comparisons between actual data and the ANFIS outputs have been



**Fig. 3.** Training error during the training of ANFIS model for estimation  $\varepsilon_2$  (a) and  $\varepsilon_4$  (b).

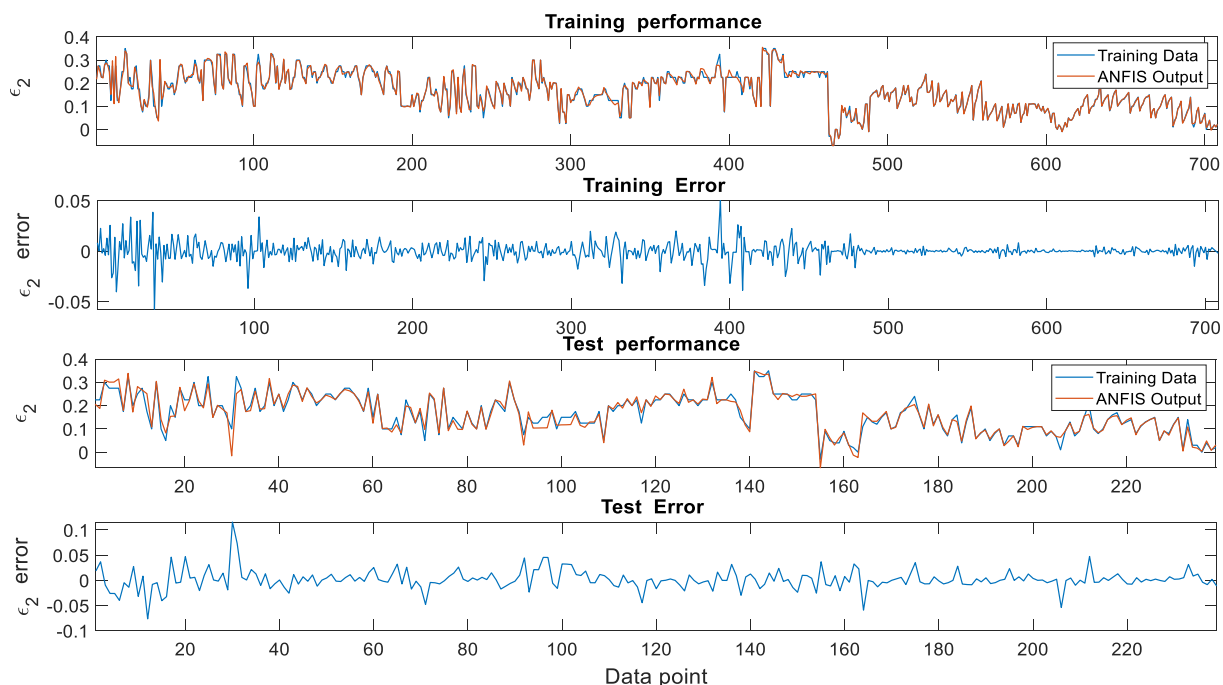


Fig. 4. The performance of ANFIS method on estimating  $\epsilon_2$  for training (upper) and test (bottom) stages.

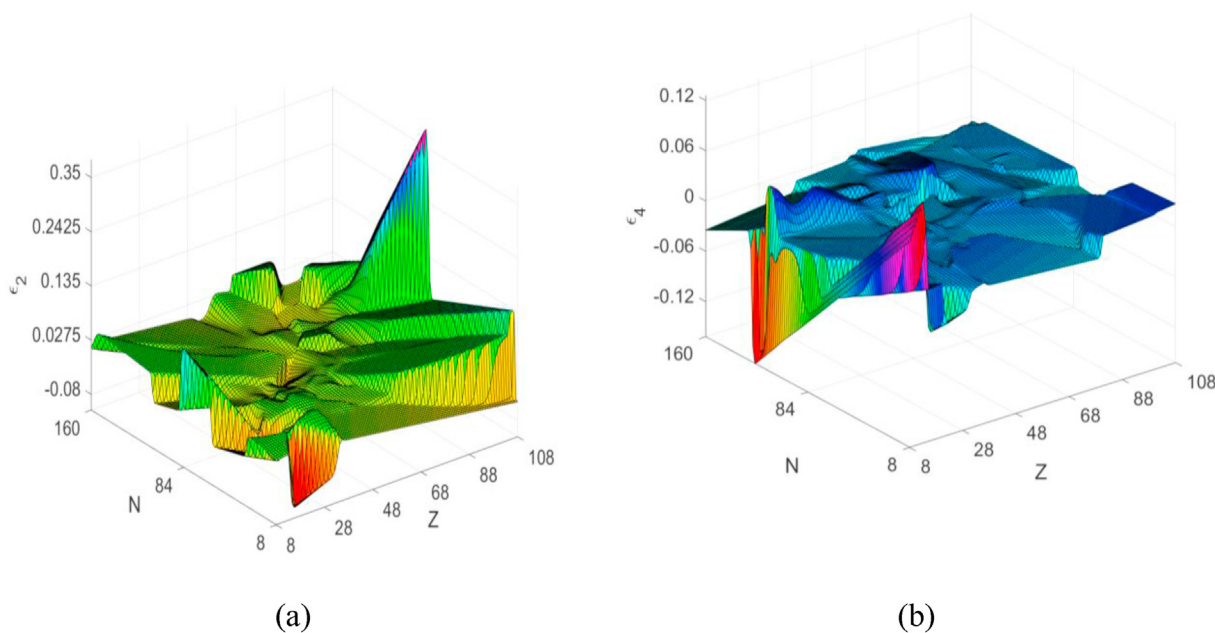


Fig. 5. The ANFIS model surface for estimation of  $\epsilon_2$  (a) and  $\epsilon_4$  (b) values according to atomic (Z) and neutron (N) numbers of the nuclei.

Table 2

The calculated performance indices for estimation  $\epsilon_4$  in the training and test phase in each fold.

$\epsilon_4$	Fold 1	Fold 2	Fold 3	Fold 4	Fold 5	Mean	StD
Test RMSE	0.0061	0.0072	0.0111	0.0105	0.0153	0.0100	0.0036
Train RMS	0.0037	0.0052	0.0030	0.0039	0.0049	0.0041	0.0009
Test MAE	0.0048	0.0050	0.0061	0.0069	0.0073	0.0060	0.0011
Train MAE	0.0027	0.0032	0.0023	0.0022	0.0031	0.0027	0.0005

explicitly shown by the figures together with the corresponding error values. As is clear in the figure that the ANFIS outputs are highly compatible with the non-linear literature data. The differences between literature data and ANFIS output are concentrated around the 0 line by getting maxima as about 0.03 and 0.05 for training and test data sets, respectively. In Fig. 5 b, the newly generated  $\epsilon_4$  values for the nuclei have been shown in the 3d graph. Clearly seen in the figure that the hexadecapole deformation parameters get the maximum (0.12) and minimum (-0.12) values at the light nuclei regions.



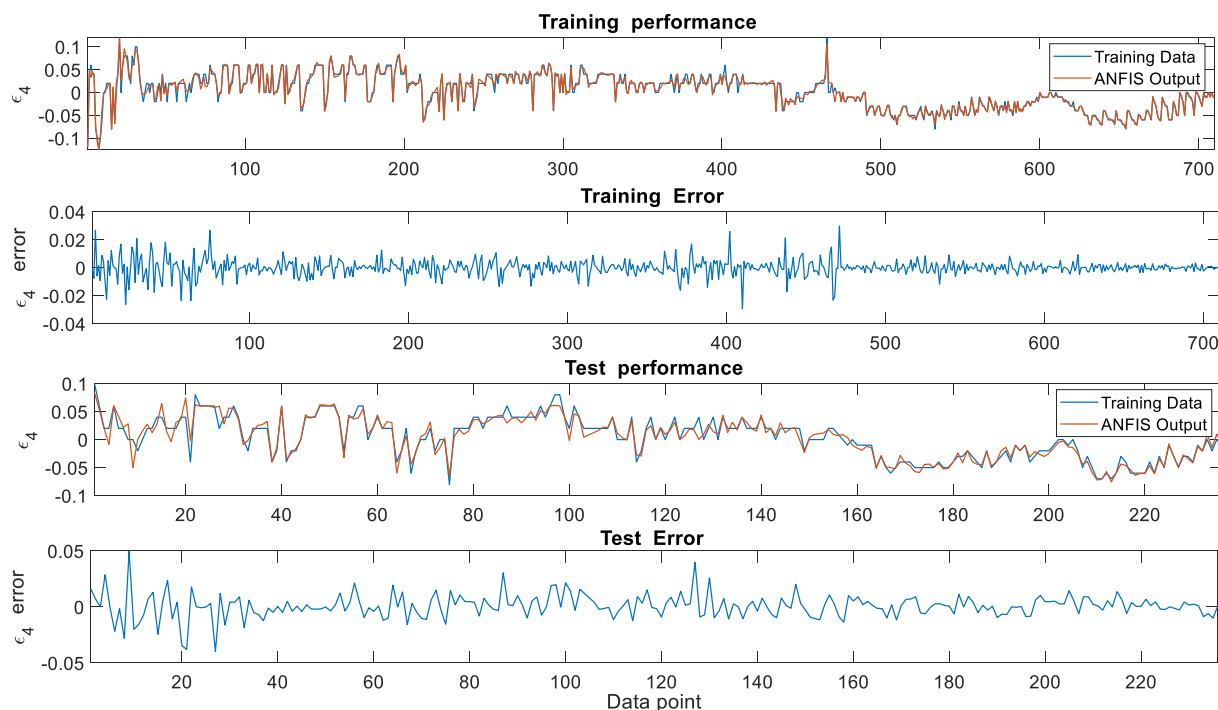


Fig. 6. The performance of ANFIS method on estimating  $\epsilon_4$  for training (upper) and test (bottom) stages.

#### 4. Conclusions

In this study, the quadrupole ( $\epsilon_2$ ) and hexadecapole ( $\epsilon_4$ ) deformation parameters for the atomic nuclei have been estimated by using ANFIS. In the calculations,  $\epsilon_2$  and  $\epsilon_4$  data have been used separately for axial and for reflection asymmetries. The training errors for  $\epsilon_2$  and  $\epsilon_4$  values are  $7.7 \times 10^{-3}$  and  $4.2 \times 10^{-3}$ , respectively. The mean RMSE values for  $\epsilon_2$  are 0.0118 and 0.0415 on training and test data sets. The better results have been obtained for  $\epsilon_4$  estimation by getting mean RMSE values of 0.0041 and 0.0100 on training and test data sets. The estimation errors which defined as the difference between the actual value and estimated value for each data instant for both  $\epsilon_2$  and  $\epsilon_4$ , are also shown in order to prove the approximation capability of the proposed method. According to the results, the ANFIS method is suitable for the estimations of quadrupole and hexadecapole deformation parameters for the nuclei which are important for the fusion-barrier distributions. Since the estimation of deformation parameters could be regarded as a nonlinear approximation problem, the ANFIS method can be used as a powerful tool for other nuclear energy-related estimation problems.

#### Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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