Predictive modeling of Young's modulus for alpha alumina using artificial neural network and multiple linear regression

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***Abstract*— In the present work, we have constructed a predictive model for one of the important mechanical properties in the study of the mechanical and thermal behavior of materials, this property is Young's modulus. The samples on which the experiments to determine the above property of alumina (α-Al2O3) were performed were made by Spark Plasma Sintering (SPS). The experimental results were exploited using the radial basis function (RBF) neural network model and multiple linear regression (MLR) to predict and construct the mathematical model. A comparison was made of the multiple linear regression model with the radial basis function (RBF) neural network model. Then, the two proposed models were compared with the experimental results. The study obtained showed good agreement between the experimental results and the proposed RBFNN models. But the MLR models were modest in predicting the studied mechanical property.**

Keywords*— Alumina, Spark Plasma Sintering (SPS), Neural network (RBF), Multiple linear regression (MLR).

I. Introduction

Across the behavioral science disciplines, multiple linear regression (MLR) is a standard statistical technique in the researcher's toolbox. An extension of simple linear regression, MLR allows researchers to answer questions that consider the roles that multiple independent variables play in accounting for variance in a single dependent variable. Artificial neural network (ANN) is one of the most important research areas related to the science of biology, electronics, computer science, mathematics, and engineering. It has wide application in solving complex multidimensional nonlinear problems, nonlinear mapping between several variables, and regularity synthesis from experimental data [1]. With the advancement of computational tools and ceramic materials science in recent years, the study of mechanical and thermal behavior of ceramic materials can be done based on knowledge and experience with these materials, using artificial neural network techniques. Several studies have been conducted on the study of mechanical parameters. In 2006, Necat Altinkok [2] applied the BP-ANN model to predict the tensile strength, hardness, and density of different metal matrix composites (MMCs). In 2020, D. Merayo et al constructed an artificial neural network (ANN), capable of making predictions on material density and Young's modulus with an average confidence of more than 99% and 98%, respectively whose topology and connections were improved to accelerate the training and predictive power of ANN [3].

The purpose of this study is to build a predictive model of the mechanical parameter Young's modulus due to its influence on the mechanical and thermal behavior, by developing a multiple linear regression (MLR) model and a radial basis function (RBF) neural network model. This paper describes how the MLR and RBF techniques work to develop the predictive model of a ceramic material (alumina). The mechanical parameter models are discussed using ANOVA statistical methods. To verify the presence of the desired input-output relationship, the multiple collinearity test was performed using the Pearson correlation test.

Finally, the ability of a radial basis function (RBF) neural network model to statistically predict the mechanical parameter of alumina was evaluated using the values of the correlation coefficient (R^2), mean absolute percentage error (MAPE), and root mean square error (RMSE) . which were calculated by Equations 1, 2, and 3.

$$R^2 = 1 - \left(\frac{\sum_{i=1}^{n} (t_i - o_i)^2}{\sum_{i=1}^{n} (o_i)^2} \right) \quad (1)$$

$$MAPE = \frac{1}{n} \left[\frac{\sum_{i=1}^{n} |t_i - o_i|}{\sum_{i=1}^{n} t_i} \times 100 \right] \quad (2)$$

$$RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (t_i - o_i)^2} \quad (3)$$

Where t is the predicted value and o is the output value and n is the total number of t and o value pairs.

II. Database

In this study, the data received from [4]. They were used to build the multiple linear regression models (MLR) and to train and test the artificial neural network (ANN) models. Sintering temperature (T), holding time (t), relative density (D), and grain size (Gs) were used as input parameters to determine the mechanical parameters of alumina developed by the SPS (spark plasma sintering) method.

A scanning electron microscope (SEM) is commonly used to examine the grain distribution of the samples. Figure 1 shows, for example, the effect of temperature on grain size.

The bulk density of the sintered samples was determined according to Archimedes' principle.

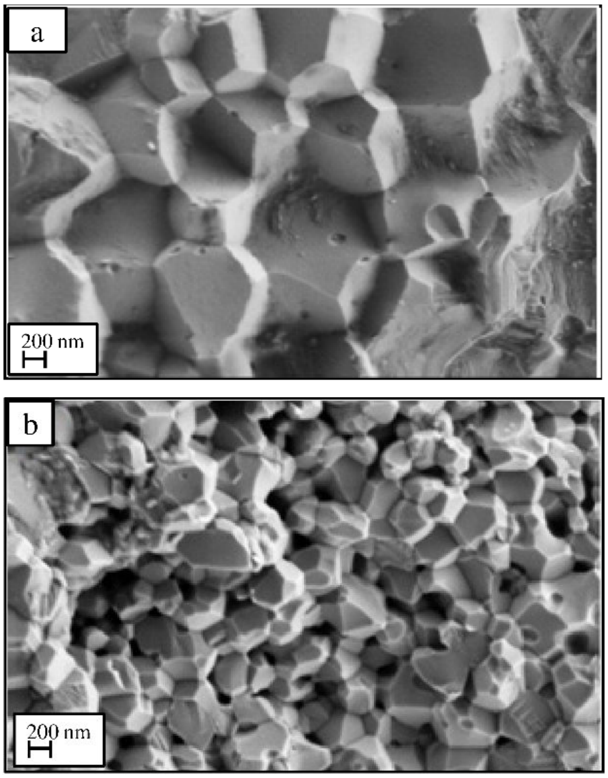

Fig. 1. Effect of processing parameters on grain size (a) and (b) effect of temperature.

Figures 2, 3 show the variation of the mechanical parameter studied in this paper as a function of density and grain size.

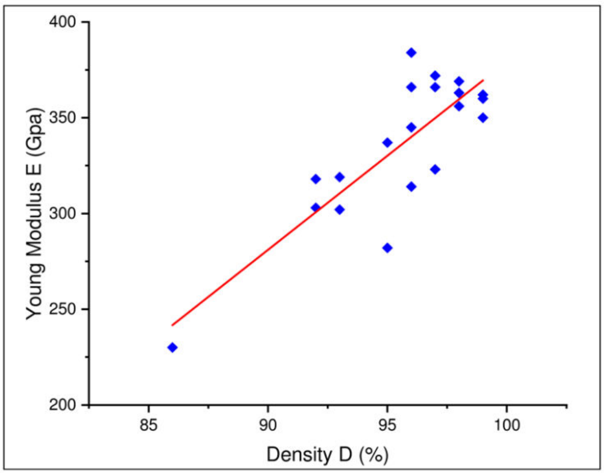

Fig. 2. variation of Young's modulus as a function of density

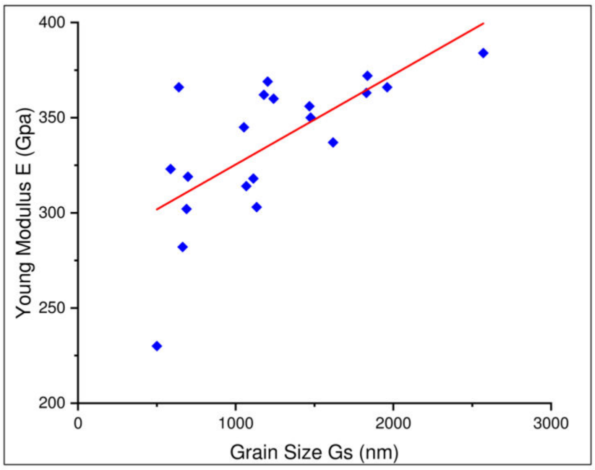

Fig. 3. variation of Young's modulus as a function of grain size

III. MULTIPLE LINEAR REGRESSION MODEL (MLR)

Regression analysis is a statistical tool widely applied in several engineering fields to model the relationship between a response variable and one or more independent variables. This modeling technique includes the statistical and mathematical approach and experimental investigations [5]. The basic multiple regression model of a dependent (response) variable Y on a set of k independent (predictor) variables can be expressed as [6]:

$$\begin{cases} y_1 = \beta_0 + \beta_1 x_{11} + \cdots + \beta_k x_{1k} + e_1 \\ y_2 = \beta_0 + \beta_1 x_{21} + \cdots + \beta_k x_{2k} + e_2 \\ \vdots \\ y_n = \beta_0 + \beta_1 x_{n1} + \cdots + \beta_k x_{nk} + e_n \end{cases} \quad (4)$$

In compacted form, equation (4) becomes :

$$y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \cdots + \beta_k x_{ik} + e_i$$

Pour *i=1, 2,…n* (5)

Where y_i is the value of the dependent variable Y for the i^{th} case, x_{ij} is the value of the j^{th} independent variable X_j for the i^{th} case, β_0 is the intercept of the regression surface, each β_j, $j=1,2\ldots k$, k is the slope of the regression surface concerning the variable X_j and e_i is the random error component for the i^{th} case.

IV. MODEL OF NEURAL NETWORKS WITH RADIAL BASIS FUNCTION (RBF)

The RBF network in it's simplest form is a back propagation neural network with three layers. The first layer corresponds to the inputs of the network, the second is a hidden layer consisting of a number of nonlinear RBF activation units, and the last corresponds to the final output of the network with a linear function. The activation functions in RBFNs are classically implemented as Gaussian functions [7]. Each layer is completely connected to the next (Fig.6). The output of the hidden layer of the network of the i^{th} activation function ϕ_i can be calculated using equation (6):

$$\emptyset_i(\|x-\mu_i\|) = exp\left(-\frac{\|x-\mu_i\|^2}{2\sigma_j^2}\right) \quad (6)$$

Here, $x = [x_1, \; x_2, \; \cdots \; x_n]$ is the input vector, $\|.\|$ is the Euclidean norm, μ_i and σ_j are the center and width of the hidden neuron j respectively.

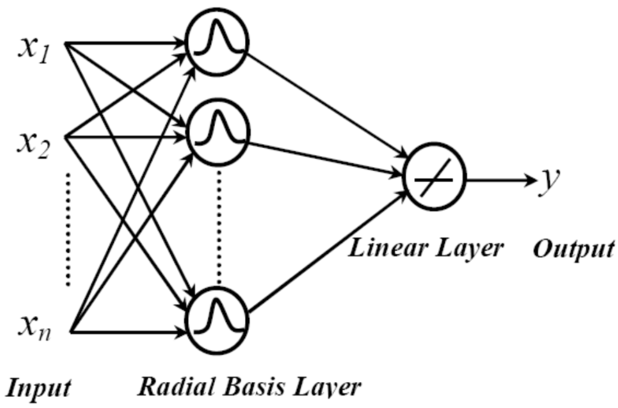

Fig. 4. Structure of the RBF neural network.

The equation characterizing the output of the RBF neural network is described by Equation (7):

$$y_i = \sum_{i=1}^{n} \omega_i \emptyset(\|x - \mu_i\|) + \omega_0 \quad (7)$$

Where μ_i the activation function centers ϕ, ω_j the synaptic weights of the network, ω_0 the bias.

V. Resultat and Discussion

A. Multiple Linear Regression Results

To find out the relationship between Young's modulus (E) and physical parameters such as density (D) and grain size (Gs) under certain experimental conditions of pressure (P), temperature (T), and time (t), the multiple linear regression model was used in which the physical and processing parameters were considered as explanatory variables and Young's modulus (E) as the dependent variable. The obtained mathematical model is studied for its statistical reliability according to the significance of the model coefficients. The statistical significance of each coefficient was checked by the probability value (P-value), and the Fisher value (F-value). A low P-value ($P \leq 0.05$) indicates statistical significance for the source on the corresponding response (i.e., $\alpha = 0.05$, at the 95% confidence level); this indicates that the resulting model is considered statistically significant, which is desirable, as it demonstrates that the terms in the model have a significant effect on the response, and higher F-values for each coefficient suggest greater significance for that term in the model [8].

The fitness of the model is measured with the R^2 value and the accuracy of the predictions is measured with the mean absolute percentage error (MAPE), which is calculated using equation (2). If the calculated MAPE is less than 10%, it is interpreted as an excellent accurate forecast, between 10% and 20% good forecasts, between 20% and 50% acceptable forecasts, and more than 50% inaccurate forecasts. An R^2 value of 0.9 or more is very good, a value greater than 0.8 is good, and a value of 0.6 or more may be satisfactory in some applications [9].

The results from the regression model showed that there was a significant relationship between and the explanatory variables. The explanatory variables explain variations in E ($R^2 = 0.845$) showing that the strength of the relationship between E and the explanatory variables is good. Referring to the value of F and its significant value P (Tab.1), we can conclude that the model is valid and that there is a correlation between E and the explanatory variables.

Thus, the results obtained give the following model equation:

$$E = 21 \times 10^{-3}T - 2{,}06t - 154 \times 10^{-3}P + 24 \times 10^{-3}G_s + 9{,}05D - 565{,}59 \quad (8)$$

To verify the existence of the mentioned relationship, a multi-collinearity test was performed, the table (Tab.2) shows the Pearson correlation coefficients between the explanatory variables and Young's modulus where the correlation coefficient was positive between Young's modulus, temperature, holding time, grain size and density. The highest correlation was for density at 0.829, followed by grain size at 0.682 and temperature at 0.610, in statistical terms, at the 0.05 significant level. The correlation coefficient with pressure and hold time was low with values of 0.146 and 0.223, respectively. The coefficients for hold time and pressure were not statistically significant.

TABLE I. ANOVA results for Young's modulus

Model	R	R^2	Variation of F	Sig. Variation of F
	0,919	0,845	15,234	0,000

TABLE II. Pearson correlation coefficients between explanatory variables and Young's modulus.

Var. explicatives	Coef. correlation	Sig. stat
Temperature (T)	0.610	0.002
Time (t)	0.223	0.173
Pressure (P)	0.146	0.269
Grains (Gs)	0.682	0.000
Density (D)	0.829	0.000

B. Modeling using neural networks (RBF)

The model was tested with different combinations of neurons in the hidden layer and it was found that the 5-17-1 model gave a better value for MAPE, RMSE, and for the correlation coefficient R^2 (Table.3).

The experimental data are grouped into training data and test data. The training data is used to train the RBFNN and the test data is used to validate the RBFNN.

Based on the prediction using the RBF model, the comparison between the predicted results and the experimental results is shown in Figure 5. As shown in Figures 5 and 6, the curves between the experimental results and the prediction results for the RBF model reveal that the RBF model has an advantage in terms of prediction accuracy and fit accuracy (99.6%).

In addition, the direct comparison of the predicted results with the experimental results is displayed using a line graph

(Fig. 6). Therefore, the RBF model produces more accurate Young's modulus prediction results.

TABLE III. PERFORMANCE PARAMETERS OF THE PREDICTED YOUNG'S MODULUS.

	Predicted YOUNG'S Modulus Performances Parameters		
	Train	Test	ALL
RMSE	1.6087	3.3051	2.0627
MAPE(%)	0.1973	0.5891	0.2757
R^2	0.999976	0.9877	0.9982

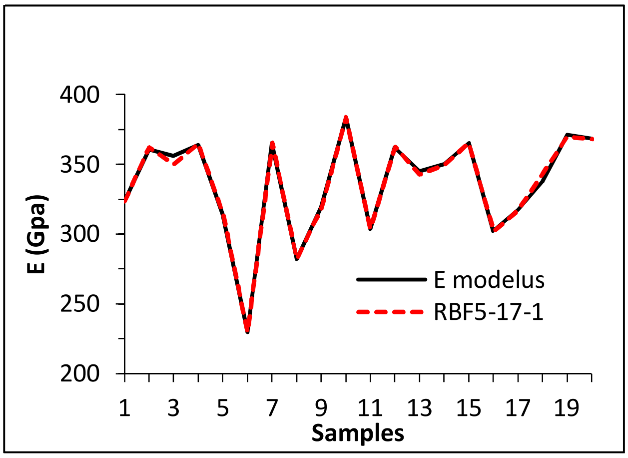

Fig. 5. Comparison between predicted and experimental results of Young's modulus.

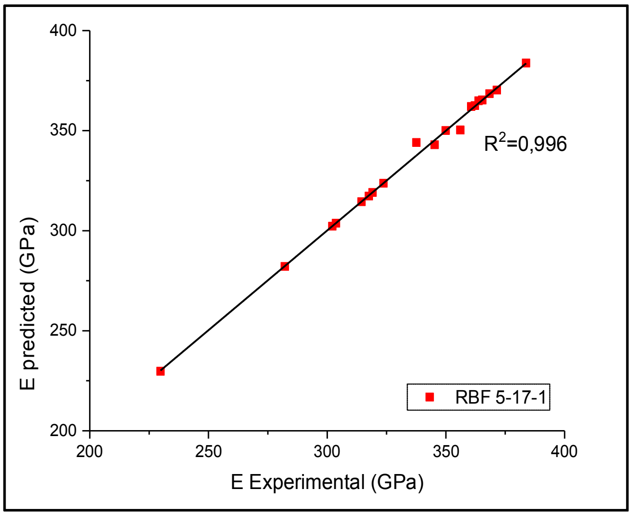

Fig. 6. Experimental and predicted values of Young's modulus.

C. Comparison of results between RBFNN and MLR

The MLR and RBFNN model predictions were compared to the experimental results for Young's modulus.

Figure 7 shows a comparison of the experimentally measured Young's modulus values and the predicted values using the MLR and RBFNN models.

It was clearly observed that the measured Young's modulus values were well correlated with the Young's modulus values predicted by RBFNN is acceptable compared to the Young's modulus values predicted by the MLR model. The minimum and maximum deviations was found for the MLR model of 0.15 and 15.28%, respectively. While the minimum and maximum deviations for the RBF model is 0 and 2.09%, the percentage error value determines the validity of the RBFNN calculation.

From the above, it is clear that the RBFNN models are suitable for predicting the Young's modulus of brittle materials especially on the studied alumina material within very acceptable error ranges. While the MLR models did not provide acceptable predictive results.

The proposed RBFNN models predict results closer to the experimental mechanical property values than the MLR models.

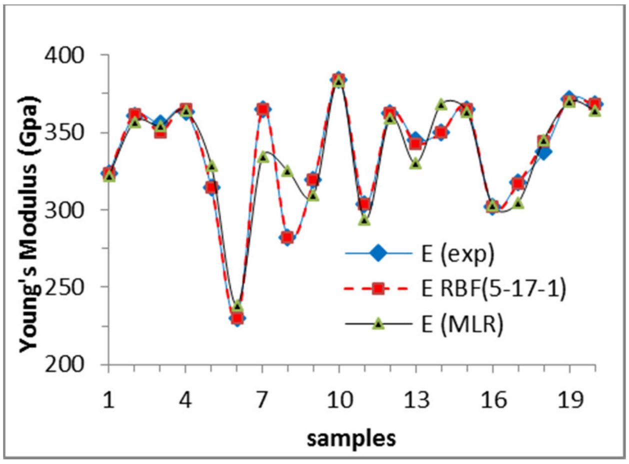

Fig. 7. comparison of predicted (MLR, RBF) and experimental results of Young's modulus.

VI. CONCLUSION

This study describes a comparative analysis of two modeling methods, namely the artificial neural network (RBFNN) and the multiple linear regression (MLR) method to predict the effect of physical properties (density, grain size) and processing parameters (temperature, pressure, and holding time) on Young's modulus of alumina.

The RBFNN model was based on 5 inputs (physical properties, processing parameters) and one output (Young's modulus) with a hidden layer of 17 neurons, and was trained using a back propagation algorithm.

Model performance was compared in terms of the predictive accuracy of the experimental results. It was found that the artificial neural network (ANN) model provided a good predictive potential for the mechanical property studied, predicting this property better than the MLR model.

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