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# Predicting the Mechanical Properties of BHA-$Li_2O$ Composites Using Artificial Neural Networks

**Hasan Huseyin Celik[1*], Oguzhan Gunduz[2,6*], Nazmi Ekren[3,6], Zeeshan Ahmad[4], Faik Nuzhet Oktar[5,6]**

[1]School of Technical Education, Department of Electronic and Computer Education, Marmara University, Istanbul, Turkey; [2]Department of Metal Education, Marmara University, Istanbul, Turkey; [3] School of Technical Education, Department of Electrical and Electronic Engineering, Marmara University, Istanbul, Turkey; [4]School of Pharmacy and Biomedical, Science University of Portsmouth, Portsmouth, UK; [5]School of Health Related Professions, Department of Medical Imaging Technics, Marmara University, Istanbul, Turkey; [6]Nanotechnology and Biomaterials Application & Research Centre, Marmara University, Istanbul, Turkey.
Email: {hcelik, oguzhan}@marmara.edu.tr

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## ABSTRACT

*In this study the mechanical properties of bovine hydroxyapatite (BHA)-$Li_2O$ composites are predicted using artificial neural networks (ANN) and then compared with obtained experimental values. BHA was mixed with lithium carbonate ($Li_2CO_3$) and sintered at various temperatures between 900-1300°C. Selected experimental values obtained for the compression strength, microhardness and density were used to define and train the ANN system. Intermediate data values not used to train the ANN model were then used to compare and determine the reliability of the ANN system. The results demonstrate the viable potential in using the ANN approach in predicting mechanical properties even with limited data sets.*

**Keywords:** *Artificial Neural Network, Hydroxyapatite, $Li_2O$ Composites, Bioceramic*

## 1. Introduction

Hydroxyapatite (HA) is an attractive material used in several hard tissue orthopedic applications. Its crystallographic and chemical properties closely resemble those of bone and tooth minerals [1]. However, because of its poor mechanical properties, HA is often used in devices as a coating, where the bioactive properties of the material can still be utilized, whilst benefiting from the mechanical properties of the substrate (e.g. stainless steel). The mechanical properties of HA, however, may be improved by additives, which can modify the sintering process, allowing the resultant material to achieve higher densities [2]. One such additive that is of interest is lithium and lithium based composites, which have demonstrated reasonable biocompatibility [3]. The relative knowledge concerning the effects of lithium compounds in such orthopedic systems on living organism is scarce; and for this reason reduced quantities of such materials must be utilized e.g. Fanowich *et al.* have utilized minimal quantities of lithium in their research (0.2, 0.4 and 0.6 wt. %) [2,4].

Artificial Neural Networks (ANN) are parallel processing models which can be deployed in predicting outcomes based on input-output data (parameters and relationships), demonstrating a degree of robustness and self-learning capability [5]. The accuracy and reliability of predicted outcomes can be increased based on the number of input values. In this way accumulation of data sets into an ANN system can enhance the outcome and predictability as the likelihood of any value will be based on previous experimental data. This makes the ANN system robust as it is an adaptive system which can change based on information it has already acquired or will obtain. This study describes the use of ANN to predict the mechanical properties of bovine hydroxyapatite (BHA)-$Li_2O$ composites. Parameters of compression strength, microhardness and density were produced by experiments in various mixture rates and temperatures. The model used was based on a feed-forward system based on sintering temperature and material composition.

BHA lithium carbonate composite, like other bioactive composites are key materials in the development of several orthopedic applications. However, sintering temperatures and compositional values for such materials occupy considerable time periods (impact on mechanical properties) and therefore the outlook provided by ANN systems can be extremely valuable. If a sufficient number of data sets can be provided then predicted data from ANN systems can suffice; reducing preliminary testing to determine mechanical properties for each type of composite or sintering temperature. In addition to orthopedics, bioceramics and their composites are also finding applications in other areas of biomaterials and biotechnologies (such as drug delivery and tissue engineering) and these predictive methods may also assist in enhancing these frontiers.

## 2. Materials and Methods

### 2.1. Materials

BHA, was prepared in similar fashion to an earlier study [6]. Lithium carbonate ($Li_2CO_3$) was purchased from (Sigma Aldrich) and was added to BHA in the compositions of 0.25, 0.5, 1 and 2 wt % $Li_2CO_3$. Ball-milled BHA- $Li_2CO_3$ powders were then pressed to cylindrical compacts (British Standard, No. 7253) which were then sintered in an open atmospheric furnace for 4 hours (Nabertherm HT 16/17, Lilienthal, Germany) at 900, 1000, 1100, 1200, and 1300°C. Density, Vickers microhardness, and compression strength were measured for all samples.

### 2.2. Mechanical Testing

Compression strength tests on sintered samples were carried out using a universal testing machine (DVT.e, Devotrans Inc. Istanbul, Turkey; speed 2 mm/min). The densities were determined using the Archimedes method and microhardness (TUKON, Wilson Instruments, Group of Instron, Darmstadt, Germany; 200 gr. load) was measured three times and a mean value was taken.

### 2.3. Artificial Neural Networks

In a feed forward ANN system, the input data is processed from input to output. The neurons are classified in three layers called input layer, hidden layer and output layer. The feed forward ANN structure is illustrated in **Figure 1.** The network input(s) and output(s) of the hidden and output layers are denoted as *Xi*, *Yj*, *Ok*. The ANN process is governed by the following equations:

$$net_j = \sum_{i=0}^{N} X_i W_{ij}^h \qquad i = 0,1,2,\cdots N \tag{1}$$

$$Y_j = f\left(net_j\right) \tag{2}$$

$$net_k = \sum_{j=0}^{M} Y_j W_{jk}^o \qquad j = 0,1,2,\cdots M \tag{3}$$

$$O_k = f\left(net_k\right) \qquad k = 0,1,2,\cdots P \tag{4}$$

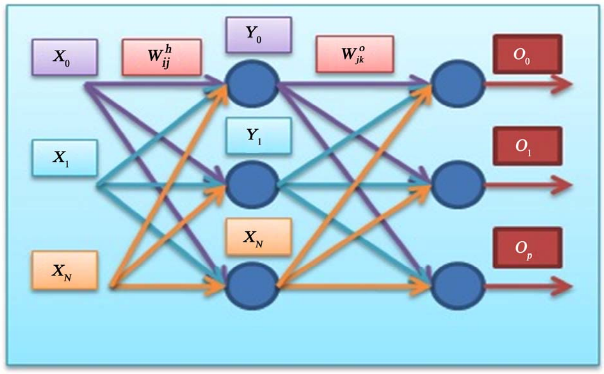



**Figure 1. Feedforward neural network architecture.**

here $W$ is weight of connections and f(.) is neuron activetion function that can be selected as hard limiter, linear or nonlinear. Because of the continuity, the activation function is frequently selected as a sigmoidal function. It can be defined as:

$$f\left(net\right) = e^{-\lambda \ net} \tag{5}$$

The parameter $\lambda$ describes the rate of the activation function. In supervised training, ANN applications require a training data set to learn the relationship between inputs and outputs. The training set should consist of sufficient number of samples that define a process. Otherwise, insufficient learning can limit the performance of the ANN approach.

## 3. Results and Discussion

Sintering of BHA-$Li_2CO_3$ composites results in the formation of BHA-$Li_2O$ [6]. **Table 1** illustrates experimental values for density, Vickers microhardness and compression strength for defined sintering temperatures and $Li_2CO_3$ compositions. For 0.25% and 0.50%, it is seen that density values increased with increments to temperature and $Li_2CO_3$ content. The highest values compression strength were obtained at 1300°C; ~73.75 MPa for 0.25% and ~75.23 MPa for 0.50%. This can be attributed to the occurrence of a glass phase, which has a wetting effect through the grain boundaries. The lowest compression strength values were observed at 1200°C; ~2.25 MPa for 1% and ~5.92 MPa for 2% $Li_2CO_3$ additions. Evidently, high amounts of $Li_2CO_3$ addition cause a decrease in compression strength. For compacts containing 0.25% $Li_2CO_3$, the Vickers hardness values increased with increasing sintering temperature. However, the same outcome was not observed for samples with 0.5, 1 and 2% quantities because of increased porosity.

Experimental values obtained for BHA composites consist of five sets of sintering temperatures (ranging from 900-1300$^o$C) and within these, properties such as density, microhardness and compression strength will

**Table 1. Mechanical Properties of BHA-$Li_2O$ composites with different $Li_2CO_3$ content.**

| T[°C] | 0.25% | | | 0.50% | | | 1% | | | 2% | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|
| | d | $\sigma$ | HV | d | $\sigma$ | HV | d | $\sigma$ | HV | d | $\sigma$ | HV |
| 900 | 2.104 | 36.02 | 41.9 | 2.816 | 56.01 | 114.89 | 2.33 | 38.43 | 59.53 | 1.742 | 15.02 | NA |
| 1000 | 2.192 | 38.64 | 53.12 | 2.826 | 57.82 | 88.24 | 2.109 | 17.13 | 65.08 | 1.661 | 12.43 | NA |
| 1100 | 2.215 | 43.11 | 62.46 | 2.852 | 59.32 | 102.45 | 2.2488 | 8.67 | 49 | 1.713 | 10.57 | NA |
| 1200 | 2.587 | 47.81 | 120.26 | 2.869 | 61.84 | 108.84 | 2.3652 | 5.27 | 51.68 | 1.651 | 8.92 | NA |
| 1300 | 2.844 | 70.75 | 175.83 | 2.758 | 72.23 | 149.09 | 2.0672 | 2.75 | 49.01 | 1.696 | 9.83 | NA |

*NA = not applicable

vary. Three temperature sets (900, 1000, 1100°C) were used to train the ANN model. A Back-propagation algorithm was used in the training process with a sigmoid type of activation function. Here, ANN models have two inputs and one output (**Figure 2**). The inputs consisted of sintering temperature and mixture rate (**Figure 3**) and the output is a predicted value (for a selected property) based on the training obtained from data provided. Training experiments were performed individually for the prediction of each property, which is now set as an outcome (density, microhardness and compression strength).

Part of the training phase is to examine the different number of neuron networks (or connections). The output value for a property (density, microhardness and compression strength) can be enhanced by increasing the number of neurons or data entry during the training stage. After the training step, the ANN was used to predict me chanical properties of the last two groups (1200 and 1300ºC) which were withheld during the training process. A comparison between the predicted (using ANN) and obtained results are illustrated in **Table 2**.

ANN based predictions of the compression strength at 1200 and 1300°C have an average maximum error rate of ~17%. Prediction error rates of density and microhardness obtained were ~7% and ~2.5% respectively. When comparing the total prediction errors of the two tested data sets (1200°C and 1300°C) , it is observed that data obtained for 1300°C is less accurate when compared to those obtained for 1200ºC, and this can be seen by comparing the predicting and corresponding values for density and compression strength. However, the reverse is

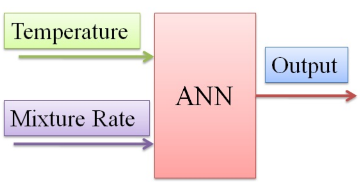
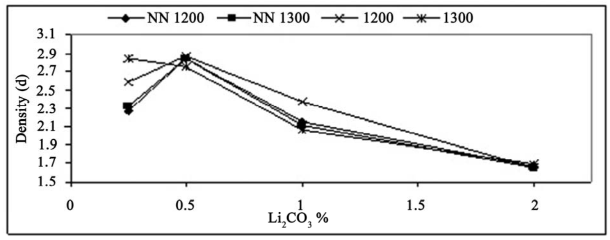
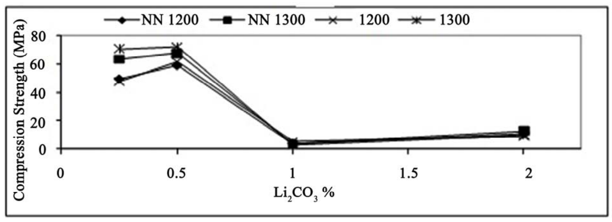


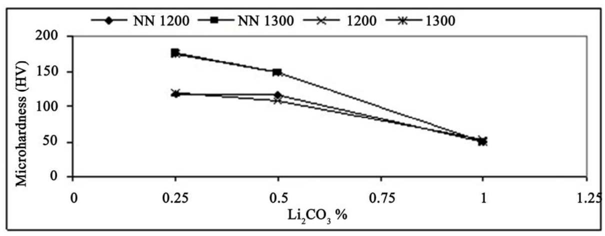

**Figure 2. Defined ANN model prediction.**




(a)




(b)




(c)

**Figure 3. ANN predicted values for a) density, b) compression strength, c) microhardness.**

true for microhardness predictions.

The results of ANN prediction for density, microhardness and compression strength are also illustrated in **Figures 3 a, b and c**; where the trend between the predicted and obtained values is clearly evident, although there are differences in the actual values.

## 4. Conclusion

According to the findings, the ANN approach can supply reasonable predicted values for limited mixture rates and temperature. Because of non-linear changes to density, compression strength and microhardness, the ANN ap-

**Table 2. Obtained values compared with ANN predictions (and relative errors).**

| | | 1200°C | | | 1300°C | | |
|---|---|---|---|---|---|---|---|
| | Mixture rate | Measurement | ANN Prediction | Relative error % | Measurement | ANN Prediction | Relative error % |
| Density(g/cm$^3$) | 0.25 | 2.587 | 2.27 | 13.96 | 2.844 | 2.32 | 22.59 |
| | 0.5 | 2.869 | 2.84 | 1.02 | 2.758 | 2.84 | 2.89 |
| | 1 | 2.365 | 2.15 | 10.00 | 2.067 | 2.11 | 2.04 |
| | 2 | 1.651 | 1.67 | 1.14 | 1.696 | 1.66 | 2.17 |
| Compression Strength (MPa) | 0.25 | 47.81 | 49.73 | 3.86 | 70.75 | 58.85 | 20.22 |
| | 0.5 | 61.84 | 59.24 | 4.39 | 71.23 | 57.69 | 23.47 |
| | 1 | 5.27 | 3.98 | 32.41 | 2.75 | 3.62 | 24.03 |
| | 2 | 8.92 | 11.09 | 19.57 | 9.83 | 12.65 | 22.29 |
| microhardness hardness (HV) | 0.25 | 120.26 | 117.63 | 2.24 | 175.83 | 177.05 | 0.69 |
| | 0.5 | 108.84 | 115.61 | 5.86 | 149.09 | 148.47 | 0.42 |
| | 1 | 51.68 | 49.654 | 4.09 | 49.01 | 49.84 | 1.67 |

proach may not provide very accurate numerical predictions for values outside of the mixture rate and temperature limits provided during training. Prediction performance can be expanded by increasing number of experimental data used in the ANN learning process. The ANN approach can provide quick predictions for mechanical properties of BHA-$Li_2O$ composites, reducing time and cost on sample preparation and analysis.

## 5. Acknowledgements

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