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# Determining boride layer thicknesses formed on XC38 steel with artificial neural network

## ABSTRACT

*Boride layers result from surface treatments of materials, offering valuable mechanical and tribological aspects that extend the material's life expectancy and potential. They are achieved by a process known as boriding in which boron atoms are diffused into the material until saturation, where a layer that may be mono or dual-phased begins to thicken over time depending on the period of treatment, the temperature held, the media applied, the composition of the material with its impurities, and more. Due to the difficulty of encompassing all those different parameters that influence the kinetic evolution of that boride layer, the idea was to start by training an artificial neural network to estimate its thickness with only two variables and inspect the results. Three experimental observations out of nine were used as validating data, while the rest were training data, along with others added. Depending on the reliability of the predictions given by the artificial neural network, further research can explore the possibilities of training it on different samples and environments through data mining.*

***Keywords:*** *Machine learning, artificial neural network, layer thickness, boride layers, boriding*

## 1. INTRODUCTION

Boriding has grown significantly as a surface treatment method for various materials, such as steels, superalloys, and other metal alloys. Researchers are continually working to optimize the processes to improve the properties of the boride layer.

Some recent studies have focused on using computational simulations to predict the evolution of the boride layer [1,2], as well as experimental investigations [3] to validate the results and understand the factors of the phenomenon. Machine learning is one of the computational techniques with great potential in predictions.

Genel et al. [4] have predicted, with high precision by an artificial neural network, the hardness and depth of the boride layer of AISI W1 steel even better than regression models. The layer of the borided steel was explored using heat treatment powder boriding at different temperatures and periods, and the analysis confirmed the existence of a two-phased layer consisting of FeB and $Fe_2B$ borides on the steel surface.

The study of Campos et al. [5] evaluated the growth kinetics of the mono-phased boride layer $Fe_2B$ in AISI 1045 steel using neural networks and least square techniques through the paste boriding process. The reliability of these techniques was compared with experimental results, resulting in mean errors of 5.31 and 3.42 %, respectively. It was concluded that the models used have the advantage of minimizing the error percentage for the thickness of the iron boride layer compared to deterministic models, which may go up to 30 %.

Liu and Zhang [6] discussed and adopted a neural network system to predict the performance of solid boriding. The system overcomes the limitations of traditional approaches and offers a stable and efficient method for predicting the diffusion layer in solid boriding.

Rayane and Allaoui [7] debated the usage of an artificial neural network technique to predict the thickness of boride layers on XC38 steel achieved through boriding treatment in different molten salts. The model provided good precision in predicting the depth of the boride layer for the different molten salts, with the highest performance attained using normalized values.

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Mebarek et al. [1] have simulated the growth kinetics of the boride layer on the same data used in this paper, XC38 steel substrate that was borided within a liquid medium, with a network of artificial neurons to predict the thickness of that boride layer and the characteristics of the kinetics of the process.

Mota-Hernandez et al. [8] provided valuable insights into the application of neural networks in materials science and engineering, where it was possible to assess the fracture toughness of borided steels. Different neural network models were analyzed and applied with errors of 5 % on both compared to experimental data of the fracture toughness of the iron boride layer.

Mebarek and Keddam [9] presented a simulation approach model based on a fuzzy neural network to estimate the thickness of FeB and $Fe_2B$ bi-phased layers in the boriding process. The model combines fuzzy logic and neural network techniques and is validated using experimental data, showing good agreement with the results obtained. While in [10], they developed a model based on the artificial neural network for the boriding process of the AISI 316L stainless steel. The developed model simulates the boriding process of the studied material, and it successfully predicted the layer's thickness with an average error of 1-1.25 μm.

In this work, a model that uses an artificial neural network is used to determine the evolution of the boride layer thickness formed on XC38 steel when borided. In doing so, an artificial neural network is given only two variables, temperature and time, and applied to nine observed layer thicknesses, along with others added, as working data from which it can predict unseen outcomes. To validate the effectiveness of those predictions and their precision, they are compared to another established model, the diffusion model [11], which uses more variables in addition to the two used in the proposed model.

## 2. ARTIFICIAL NEURAL NETWORKS

Researchers observed the human brain, the root of thoughts and learning, and focused on its foundational unit, the neuron, with its thousands of connections forming a network. As illustrated in Figure 1, a neuron receives information with the dendrites from a preceded cell and then sends it to another with its terminal after processing it. The connection between a dendrite and a terminal forms a synaptic that is dynamically strengthened or weakened based on how often it is being used [12].

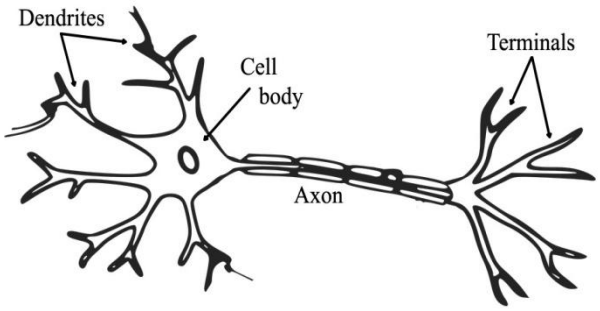


*Figure 1. Illustration of a biological neuron structure*

Each received information is referred to as an input and is weighed by that synapse's strength. The result is a bunch of information that is summed in the cell body and transformed into a signal transferred through the axon and sent to another synaptic connection or a cell as an output [12].

Inspired by that, the idea of machine learning came, where a similar structure is constructed, Figure 2, resulting in an artificial neuron characterized as a transfer function or activation function that provides the desired outputs based on inputs evaluated through weights and biases. In the middle of the structure, multiple neurons can be introduced, constituting one or multiple hidden layers, each having its own bias. An output layer follows the last hidden layer, and each layer needs a transfer function to estimate the proceeded outputs [12-14].

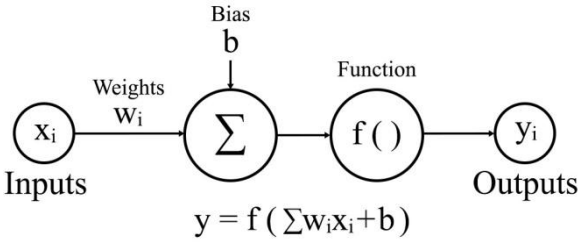


*Figure 2. Structure of artificial neurons*

Artificial neural networks differ in the connections between the neurons of each layer and the network structure. In this study, the feed-forward network back-propagation type is picked. The first part of the naming, feed-forward, is due to the absence of connections between neurons within a layer and connections that transmit data between layers in the opposite direction [14], while the second part, back-propagation, is due to a computation of the steepest gradient descent, which helps find the minimum error by adjusting weights in the direction that minimizes the overall error [12].

Following the structural choice, the training function is picked where two types were investigated, the Levenberg-Marquardt and the Bayesian Regularization functions [12]. Between both, the Levenberg-Marquardt function gave decent results in terms of mean squared errors, while sometimes it gave unfitted results. Additionally, its predictions were shifting a lot from one training to another. On the other hand, the Bayesian Regularization gave the finest and fittest results while staying stable in each execution. Both methods use the Jacobian for calculations, for which the performance function was set as the mean squared error (MSE).

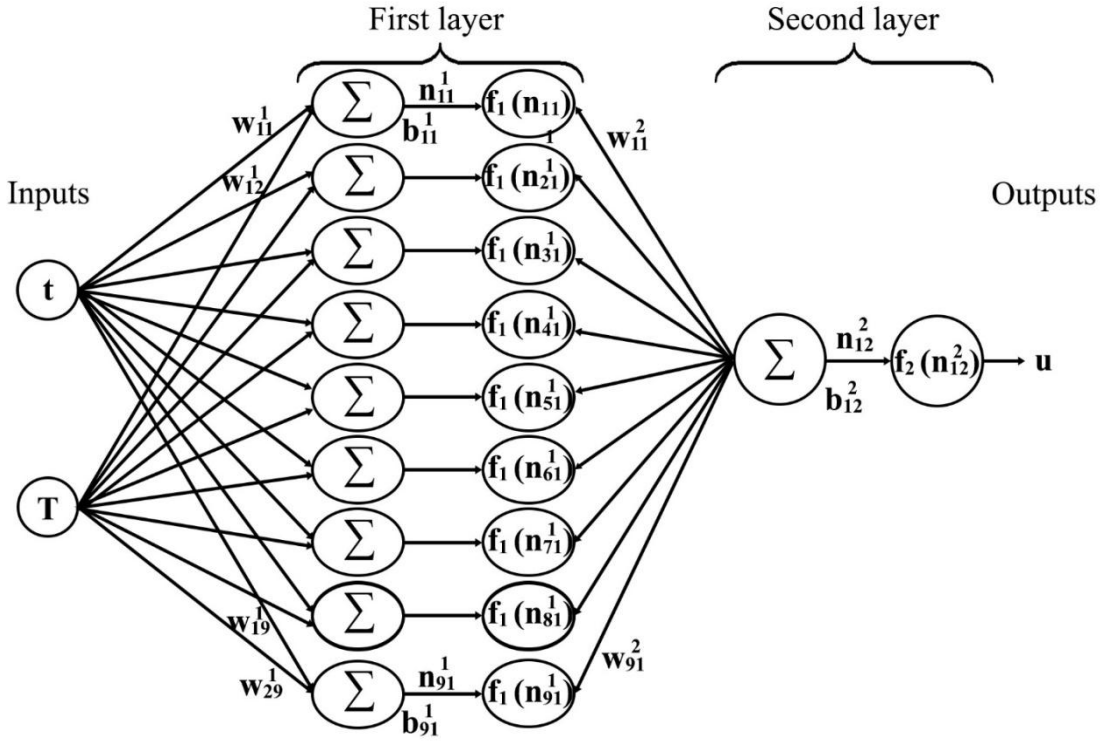


*Figure 3. Schematization of the trained artificial neural network*

For the training, two layers were computed, the last as an output layer and the first being the hidden layer with a different set of neurons. The transfer functions used in the layers were the Sigmoid function, equation (1), from the hidden layer to the output layer, and the Linear function, equation (2), from the output layer to the outputs. Furthermore, by using both functions, the artificial neural network weighs two inputs, treatment time t and temperature T, and then, with its structure, it estimates a single output, the boride layer thickness u. Within the hidden layer, different sets of neurons give different results, from bad to great predictions, but after trial and error, an optimal set can be achieved. In this case, the optimal configuration was with nine neurons, as illustrated in Figure 3.

$$f_1(n) = \frac{1}{1+e^{-n}} \quad (1)$$

$$f_2(n) = n \quad (2)$$

## 3. EMPIRICAL DATA

After establishing the structure and the parameters of the artificial neural network, it is given data to train on. The data provided were those of boriding processes experimented on an XC38 steel. The process had nine experimentations, 2, 4, and 6 hours of treatment times, each at different temperatures, 850, 950, and 1000 degrees Celsius. At the end of each process, with a light microscope, the boride layer thickness was determined [11], Figure 4. In addition to those nine observations, four others were added, the beginning of experiments having nonexistent boride layer thicknesses, from 850 to 1000 by 50 degrees Celsius, resulting in thirteen data sets.

Subsequently, three of the nine observed data, 2, 4, and 6 hours at 950 degrees Celsius were used as validating data, while the rest were training data. The artificial neural network estimates its performance by validating data and takes the best weights and biases for hyper-tuning to establish the model.

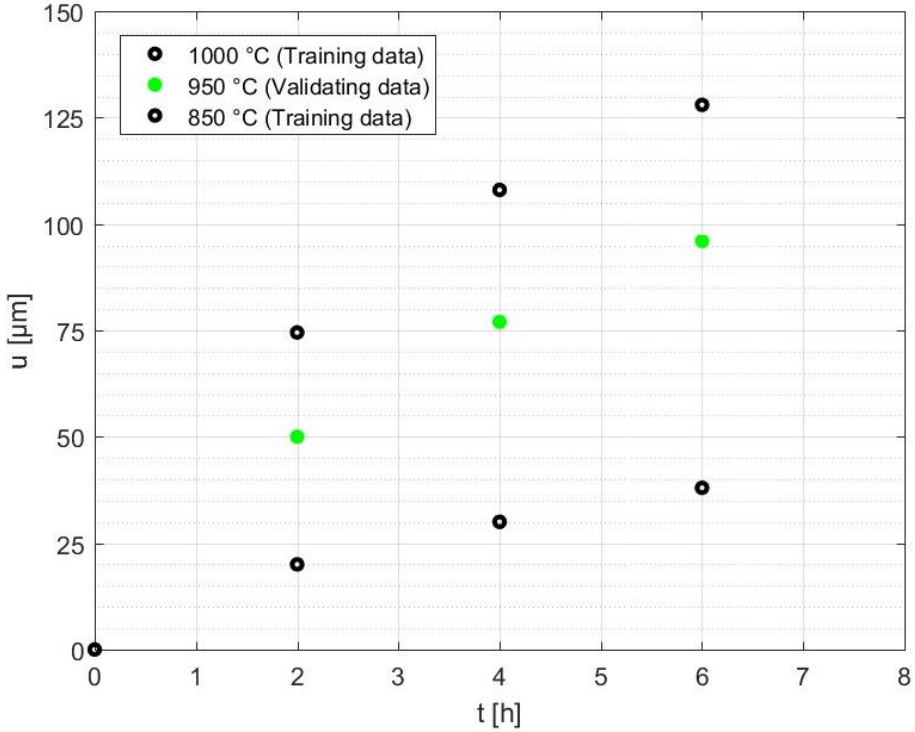


*Figure 4. Data of the empirical boride layer thickness with respect to temperature and time [11]*

## 4. RESULTS

After establishing the parameters that the artificial neural network relies on to edify itself and the data inputs and outputs that it trains and validates with, it has been launched on a thousand epochs for each set number of neurons, finding, as stated previously, the nine-neuron configuration having the best results, Figure 3.

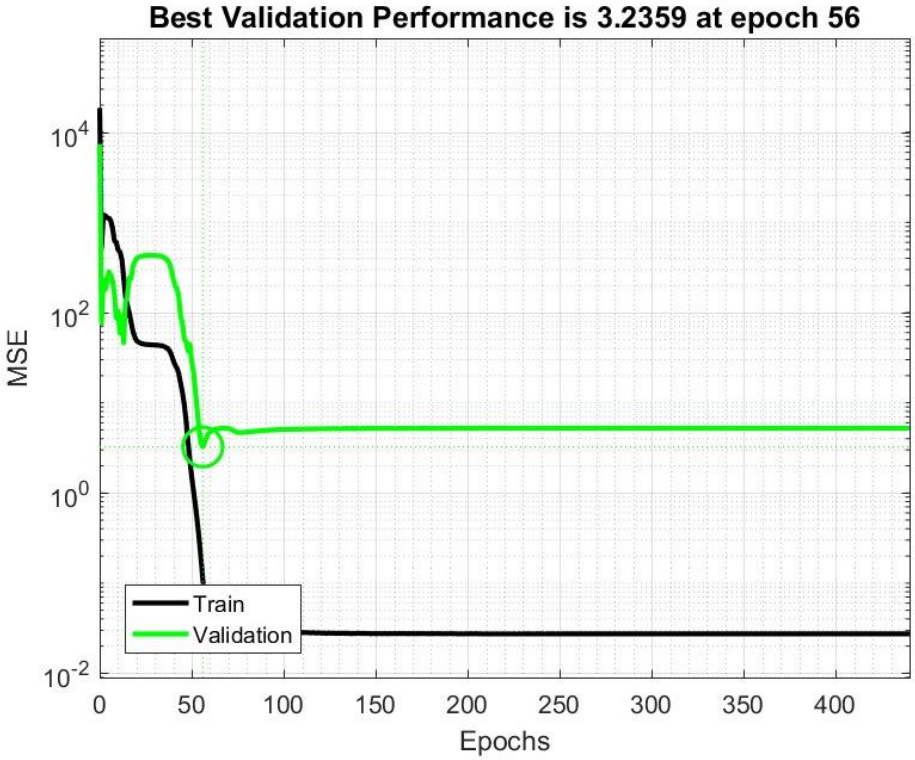


*Figure 5. Performance plot of the mean squared error*

As of all artificial neural network training, as elucidated in Figure 5, in the given epochs, the gradient decent at the beginning under the hundredth epoch of the training is remarkable, which means that the artificial neural network is adapting to the data. Following that, it stabilizes, and in the 56th epoch, there is an alteration, and the best validation performance is reached.

After training the artificial neural network, it is given two inputs, time $t$ and temperature $T$, from which it determines the boride layer thicknesses accordingly. The predictions are enumerated in Table 1, with those of a diffusion model published in a previous research paper [11], to test whether the specified trained artificial neural network is comparable.

*Table 1. Boride layer thickness values of both models*

| **T [°C]** | **t [h]** | | |
|---|---|---|---|
| | 2 | 4 | 6 |
| 850 | 23.41 | 33.11 | 40.55 |
| 950 | 53.22 | 75.26 | 92.17 |
| 1000 | 76.68 | 108.44 | 132.82 |
| **[µm]** | $\mathbf{u_D}$ | | |
| | $\mathbf{u_A}$ | | |
| 850 | 20.20 | 29.72 | 38.12 |
| 950 | 52.72 | 77.33 | 94.51 |
| 1000 | 73.88 | 108.45 | 127.49 |

From the given results of Table 1, the results of the boride layer thickness obtained from the trained artificial neural network $u_A$ seem close to those of the diffusion model $u_D$.

Consequently, an extrapolation of the trained artificial neural network is investigated by plotting, as in Figure 6, the diffusion kinetics throughout the treatment time.

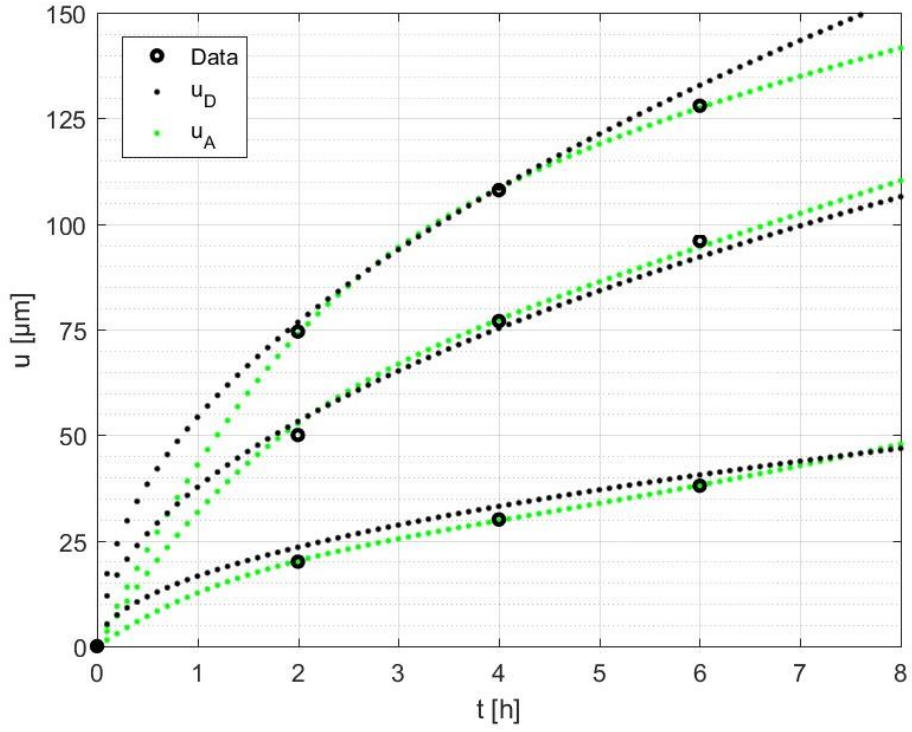


*Figure 6. Simulation of the boride layer thickness over time in both models*

Extrapolating the artificial neural network's predictions from the beginning until 8 hours of treatment provided promising results, more favorable than those of the diffusion model, as seen in Figure 6. Hence, it can be said that the artificial neural network has the potential to describe the kinetics of boride layer thicknesses even though it used only two variables, time $t$ and temperature $T$. Moreover, the predictions of each model's residuals are provided in Figure 7.

## 5. RESIDUAL ANALYSIS

This section is dedicated to the accuracy difference between both models regarding the empirical data, where a better perception of their conformity is given, along with two statistical metrics. The first metric is the mean squared error (MSE), equation (3), where we can get the average squared loss between the estimated boride layer thicknesses and the experimental ones. The second metric is the mean absolute error (MAE), equation (4), which is generally less sensitive to one or two significant errors in the data set, making it more robust to outliers than the mean squared error [12].

$$MSE = \frac{1}{n}\sum_{i=1}^{n}( u_i - \hat{u}_i )^2 \quad (3)$$

$$MAE = \frac{1}{n}\sum_{i=1}^{n}| u_i - \hat{u}_i | \quad (4)$$

Where: $u_i$ experimental layer thicknesses, $\hat{u}_i$ estimated layer thicknesses, $n$ data set number.

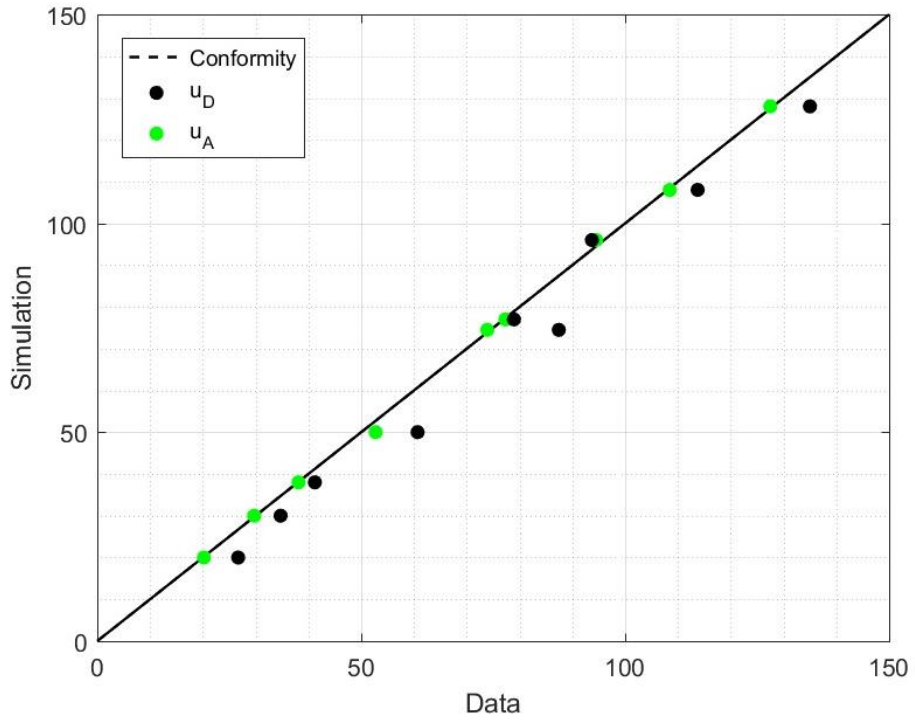


*Figure 7. Graph of conformity between both models and the experimental data*

With each model's simulated boride layer thicknesses plotted against the actual experimental data in Figure 7, it is seen that the artificial neural network's estimations conform better than those of the diffusion model to the experiments, and in consequence, the validation of the efficiency of the artificial neural network model regarding the observed experiments.

Other than that, the starting data points when the treatment time is null are ignored for the statistical metrics, and two comparisons are given: the first being the nine experimental data and the second only the validating data (the three empirical points of the 950 degrees Celsius).

Table 2 presents that if a comparison were to be done using the experimental data points, all the statistical metrics would be way better in the artificial neural network due to the training of the artificial model on the non-validating points, i.e., the other six observed data. Thus, taking only the three validating data would be less biased, and even with that, it is clear that the artificial neural network performs nearly twice as well as the diffusion model in both the statistical metrics measured.

*Table 2. Accuracy metrics for both the artificial neural network and the diffusion model*

| | All data points | | Validating points | |
|---|---|---|---|---|
| **[µm]** | **MSE** | **MAE** | **MSE** | **MAE** |
| $\mathbf{u_D}$ | 9.335 | 2.811 | 9.337 | 2.927 |
| $\mathbf{u_A}$ | 1.176 | 0.746 | 3.236 | 1.512 |

## 6. INPUT-OUTPUT RELATIONSHIP

Lastly, the trained artificial neural network is used to cover the inside of the studied domain of data, from 850 to 1000 degrees Celsius for two to six hours of treatment time, in a three-dimensional graph, Figure 8, of the boride layer thickness as a function of temperature and time to see if the artificial neural network could cover the relationship between the variables, inputs, and the results, outputs, by providing correct material science insights.

After obtaining the resulting domain, the empirical data are scattered within it, as seen in Figure 8. For a relationship breakdown between the inputs and outputs, three more graphs of each side view of the 3D graph are illustrated in Figures 9, 10, and 11.

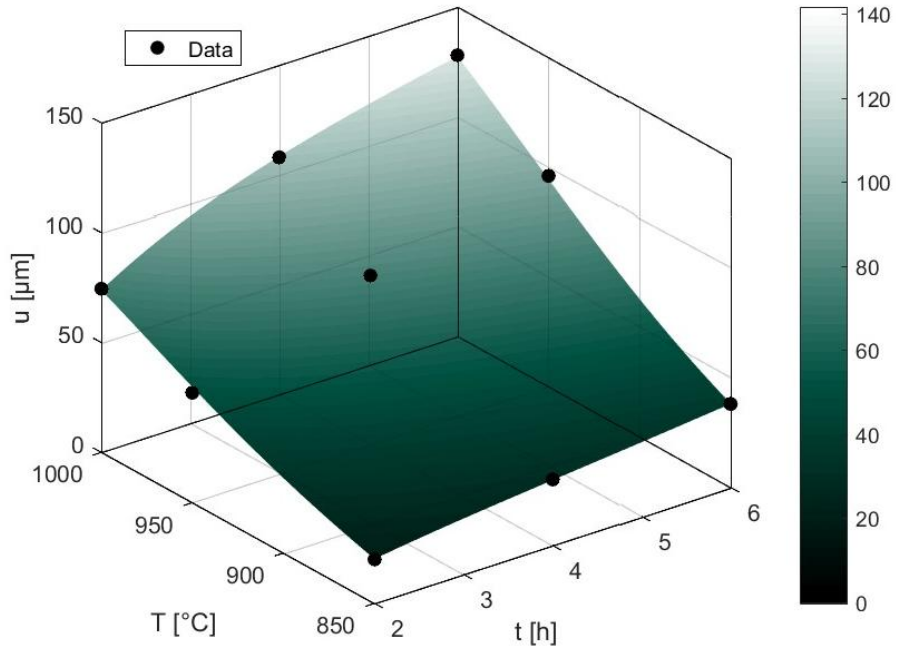


*Figure 8. 3D predictions of boride layer thickness in a domain of 2 to 6 h at 850 to 1000 °C*

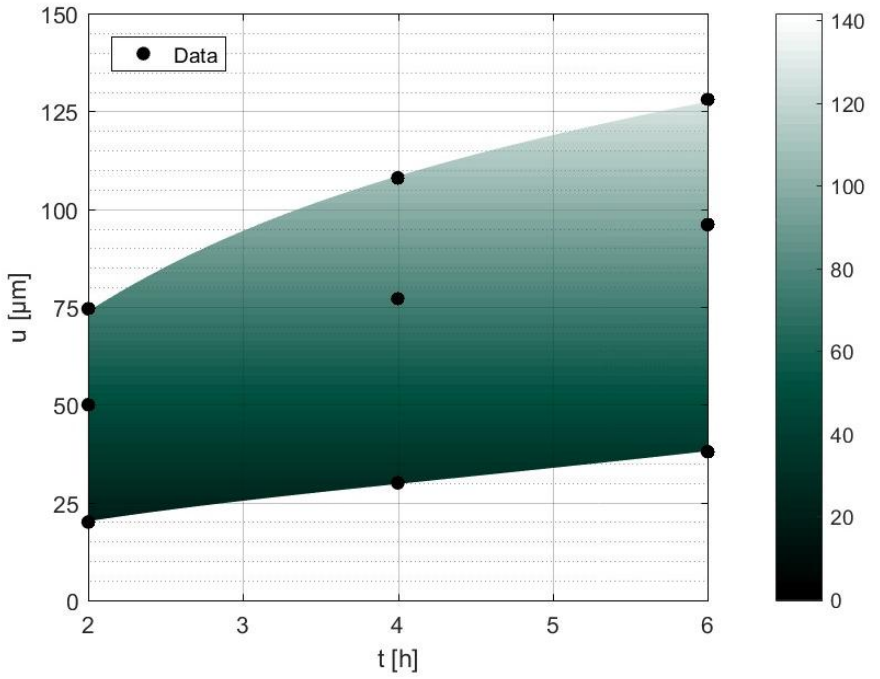


*Figure 9. Boride layer thickness against time in a side view of the predicted domain*

The first side view, Figure 9, resembles the one in Figure 6, where the kinetic of the boride layer thickness is represented over time. It can be seen that there is a slow, nearly linear evolution of the boride layer thickness at the lowest temperature (850 degrees Celsius). In comparison, in the highest temperature (1000 degrees Celsius), the evolution at first is notable but decreases over time. Those evolutions confirm the initial influence of the temperature in the first stages of the diffusion of the boron atoms into the substrate, where the boride layer thickness increases rapidly in high temperatures compared to lower ones. However, over time, both evolutions seem to linearize.

The second side view, Figure 10, portrays slight inaccuracies in the middle with the empirical data and characterizes the impact of the time on the boride layer thickness. The extremes of the domain, the bottom and upper limits, represent two and six hours of treatment times at different temperatures, respectively.

For a fixed temperature in Figure 9, the evolution of the boride layer decreases over time, unlike in Figure 10, where the evolution of the boride layer increases for a fixed treatment time. Thus, it can be said that the temperature has a more significant influence than the treatment time.

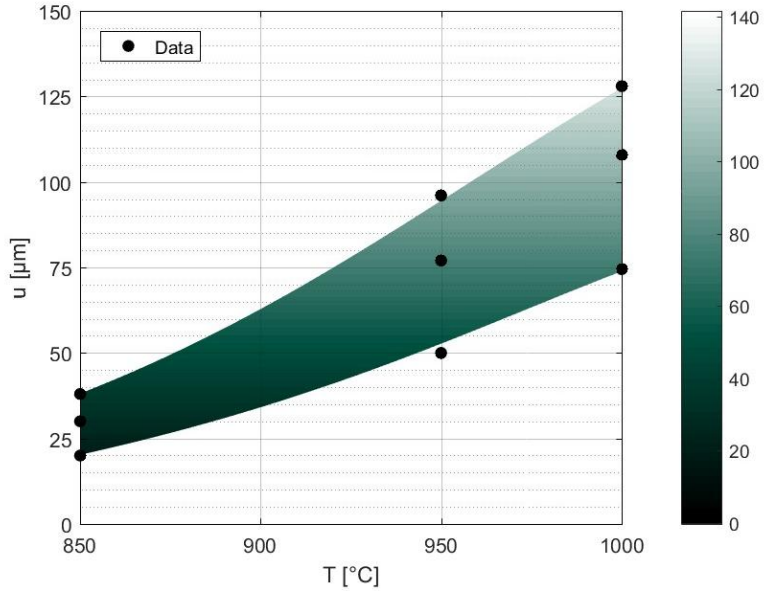


*Figure 10. Boride layer thickness against temperature in a side view of the predicted domain*

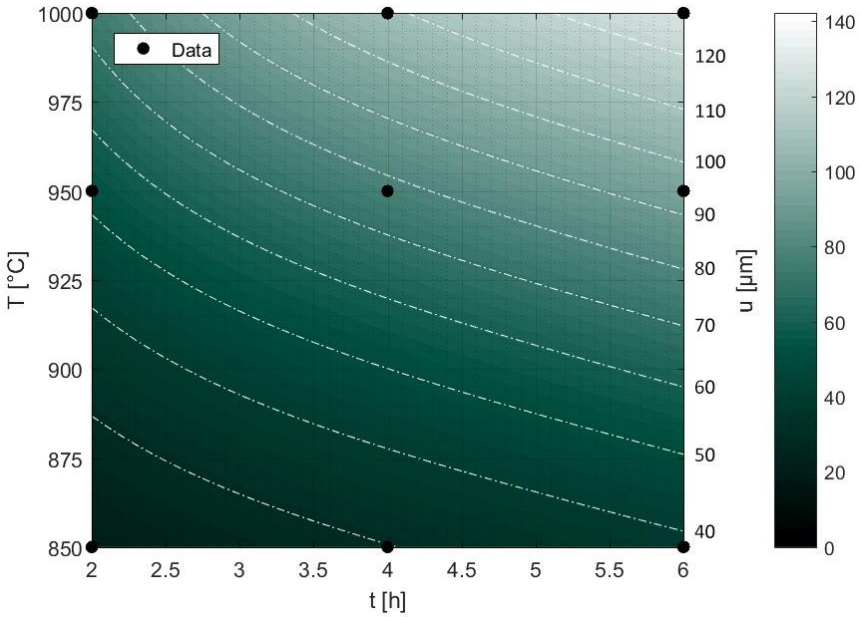


*Figure 11. Evolution of the boride layer thickness in an iso thickness diagram*

From the top view, Figure 11, the graph gives different boride layer thicknesses for each chosen temperature and time, known as the iso-thickness diagram. It is consistent with the literature, where for a fixed boride layer thickness, temperature decreases with the increase of the treatment time. As an example, highlighted in white at the bottom of the graph, boriding for 4 hours at 850 degrees Celsius gives roughly the same boride layer thickness as boriding for 2 hours at nearly 885 degrees Celsius.

## 7. CONCLUSION

Training functions used by artificial neural networks are not all suitable for training on the kinetics of the boride layer thicknesses. This inference was reached from the trial and error in establishing the model, where it was observed that the Levenberg-Marquardt function gave approximate results in some executions but diverged in most others, contrary to the stability and accuracy of the Bayesian Regularization function.

Knowing that the phenomenon is not chaotic and has physical sense, taking limited data points can be sufficient, as it has been shown, where despite taking only two variables, the determination of the boride layer thickness was comparable to the diffusion model, which uses more variables to be established.

In contrast, the artificial neural network grasped the relationship and impact of the variables, representing the temperature's influence as more significant than that of the treatment time. Additionally, it can even provide the iso-thickness diagram, which is an essential industrial graph.

Moreover, the artificial neural network has the potential to significantly contribute to the kinetic studies of boride layers due to its observed performance in predicting their thicknesses. Thus, further investigations can be carried out on other data substrates with mono-phase Fe2B and dual-phase FeB/Fe2B layers or even variables such as boron content, hardness, wear, and others, depending on the availability of the empirical data.

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## IZVOD

### ODREĐIVANJE DEBLJINA BORIDNOG SLOJA FORMIRANOG NA ČELIKU XC38 SA UMETNUTOM NEURONSKOM MREŽOM

*Boridni slojevi su rezultat površinske obrade materijala, nudeći vrijedne mehaničke i tribološke aspekte koji produžuju životni vijek i potencijal materijala. Oni se postižu postupkom poznatim kao borenje u kojem se atomi bora difundiraju u materijal do zasićenja, gdje sloj koji može biti jednofazni ili dvofazni počinje da se zgušnjava tokom vremena u zavisnosti od perioda tretmana, održane temperaturi, medija primijenjen, sastav materijala sa njegovim nečistoćama, i još toga. Zbog poteškoće da se obuhvate svi oni različiti parametri koji utiču na kinetičku evoluciju tog boridnog sloja, ideja je bila da se počne obučavanjem veštačke neuronske mreže da proceni svoju debljinu sa samo dve varijable i pregleda rezultate. Tri eksperimentalna zapažanja od devet korištena su kao validacijski podaci, dok su ostali bili podaci o obuci, zajedno s ostalim dodanim. Ovisno o pouzdanosti predviđanja koje daje umjetna neuronska mreža, daljnja istraživanja mogu istražiti mogućnosti njezine obuke na različitim uzorcima i okruženjima kroz rudarenje podataka.*
***Ključne riječi:*** *Mašinsko učenje, umjetna neuronska mreža, debljina sloja, boridni slojevi, boronizacija*

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