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Deep Neural Networks in Processing of MoOx with fsLaser Pulses

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Abstract. Artificial Neural Network (NNs) approaches allow for the automatic creation of a model that accounts for these challenging processes, without any physical knowledge of the processes being programmed by a specialist. Fs short-pulse lasers can be used to create oxides in any type on materials, but to model such interactions requires expensive techniques. Multilayer neural networks allow one to take a relatively sparse ensemble of simulations and generate a surrogate model that can be used to rapidly search the parameter space of interest. Whereas traditional machine learning (ML) algorithms (such as Random Forests) may saturate with respect to their capabilities with substantial amounts of data, NNs seem to continue to improve as data increases. In this work an artificial neural network is trained in Python language using the Keras and Tensorflow tools, using the Adam optimizer and with a set of 8000 training epochs. The input variables are the parameters of ultrashort femtosecond pulses irradiating a molybdenum metal layer.

Keywords: Metal laser processing, deep neural networks, molybdenum oxides.

1 Introduction

The processing of materials with pulsed femtosecond lasers with very high repetition rates in the order of 60MHz is a complex process that generates non-linear absorption in the material, the short duration of the pulses of a few femtoseconds allows generating very precise microstructures on the surface, controlling their spatial resolution. Experimental optical setup of material processing with fs pulsed laser in Molybdenum thin films is show in Fig. 1a [1]. Consequently, in Fig. 1b each fs pulse, in conjunction with the high repetition rate, removes a minimal amount of material with minimal

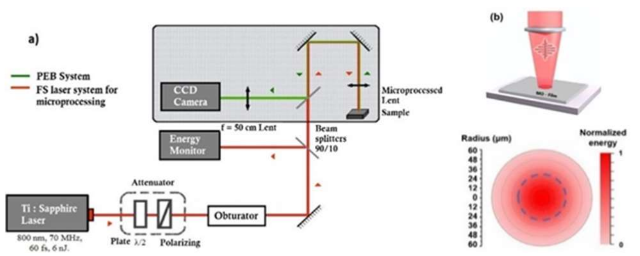

Fig. 1. (a) Experimental optical setup of material processing with fs pulsed laser [1], (b) Radial transformation on the surface of the film when interacting with fs pulses laser.

Fig. 2. Data processing through deep learning.

thermal damage, allowing for unmatched depth control and radialtransformation on the surface MoO_x.

The interest of generating metal oxides using ultrashort pulsed lasers offers the advantage of miniaturizing designs or crystalline structures of a specific MoO_x by controlling the heat affected zone and micrometric dimensional precision, thus the surface of the film is clean. Developments in machine learning promise to ameliorate some of the challenges of modeling complex physical systems through neural network based surrogate models [2].

There are exist simulation techniques with Deep Learningthat allow to reproduce energy curves, electron temperature, time functions, among others. Obtaining and predicting these oxides by means of learning layers has an impacton the understanding of the phenomenon that persists when irradiating a thin layer of Molybdenum.

This work focuses on the creation of a deep neural network, able to predict results of experimentation generated by 60 fs laser pulses by influencing a 500 nm of thickness molybdenum slim layer [1]. In Fig. 2, we can see the sequence used, beginning with the data input, its processing and normalization necessary for network training, and finally the result obtained from the prediction.

By the deep learning use, simulates the behavior of the fs pulsed laser in the metallic surface of the molybdenum layer where experimentally the MoO_x are obtained depending on the laser parameters, exposure time and the properties of the metallic film. The advantage of using ultrashort pulsed lasers is that offers a fine control in the formation of molybdenum oxides in localized regions and micrometric scales [1].

The data used is preprocessed and augmented to train an accurate network on the output parameters and once the results are obtained, the necessary adjustments are made to obtain an optimal response [2]. Mainly, it seeksto establish a data analysis base to make increasingly complex networks including analysis of experimental images through which each of the types of oxide present can be identified.

Table 1. Set of experimental data prepared for the study.

Fluence (mJ/cm^2)	Time (s) 2	10	20	30	60	180	360	600	1200
0.5	0	14.1	13.05	16.1	26.84	41.05	45.68	48.52	59.26
0.7	19.57	41.57	55.78	65.26	74.42	80	86.42	90.1	96.1
0.9	43.68	76.31	83.57	84.63	85.47	88.84	92	96.1	105.89
1.1	82.73	90.52	92.84	93.89	93.68	95.26	100	101.57	104.21
1.3	80	94.73	98.1	97.89	98.31	99.15	101.68	104.73	107.57
1.5	86.63	98.1	98.21	99.15	99.26	101.15	104.42	104.21	101.05

2 Data Analysis

The used data set in the neural network conforms by 60 elements of experimentation, showed in the Table 1, this information was allowed in three columns ordained by diameter, fluence and time. The resulting database is a table with 3 columns and 55 rows from which the trainingparameters for the neural network are obtained.

The data is sorted and separated by commas, so the file ending is CSV. We use data augmentation, a standard technique indeep learning. The data set was increased by a simple cubic interpolation by a factor of 2, resulting like it's shown in Fig. 3 obtaining 120 data of these process.

3 Neural Network Architecture

Establish the architecture of the neural network, several structures were tested, the one that worked best was a network 1x64x128x64x1 with 3 input parameters: Fluence,time and experimental diameter and one output variable we obtain the predicted diameter. The data were preprocessed and normalized to be entered in a first layer andthen proceed through 3 internal layers, finally a resulting value of the final layer is obtained. The final architecture of the network is shown in Fig. 4.

4 Training and validation

For this project, supervised learning was used by which the neural network was trained. The adaptive moment estimation (Adam) was used for the optimizer and the MSE for the loss function [2]. The neural network was trained for 8000 epochs, using Keras backend API Keras-TensorFlow v2.9.0, which took the computer around 24ms to complete an epoch on a machine with AMD Ryzen 5 4500U CPU with Radeon Vega6 iGPU, without using the GPU before the CPU, using the Python 3 language, for a total time of 4 minutes for the complete training of the algorithm.

The training is done using the basic linear regression formula applied by TensorFlow [3] for regression models as:

$$y = \beta + \alpha x + \varepsilon. \tag{1}$$

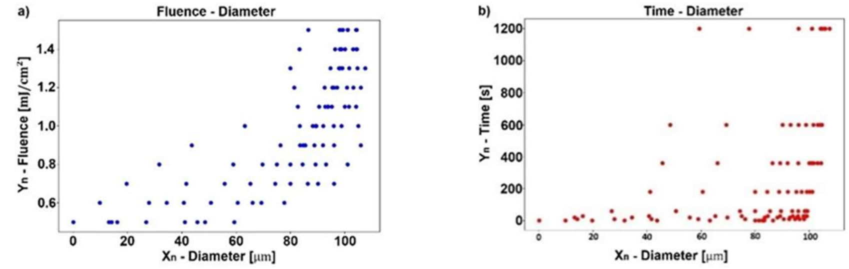

Fig. 3. Representation of scatter diagrams applying the increase of data through simple quadratic interpolation [2], a) Laser fluence in relation to the diameter, b) Exposure time inrelation to the diameter [1].

In which β is the bias, that is, if $x = 0,\ y = \beta$; α is the weight associated with x and ε is the residual or error of the model, which includes the data that the model cannot learn. Applying this formula to our case, it would be:

$$\sum diam_{pred} = \beta + \alpha 9 diam_{exp} + F_{pp} + t_{exp}= + \varepsilon. \quad (2)$$

With the variables related to the experimental diameter, the fluence, and the exposure time, as well as an MSE error function like the following:

$$MSE(y) = {}^{C}\mathrm{DEEE} \sum^{\mathrm{DEEE}} (predict - real\ value)^2, \quad (3)$$

where the value of 8000 is the number of epochs used in the neural network, predict refers predicted value, and real value is the reference to the training value.

Neural network was trained for 8000 epochs due to limited input data, finding at this point the best learning response. Finalizing with an overfitting in the neural network after this number of epochs and it starts to overfit suffering significant noise. With overfitting we refer to what happens to a model when it models the results of a training too well, learning details of these that are not general.

In this case, time and fluency areaffected, data used to demonstrate the relationship between the appearance of laser irradiation and the diameter of growth of the zone transformed into the thin metallic film. The learning rate and validation split was lr=0.001 and Vs=0.001 respectively. The best learning rate in general is the one that decreases as the algorithm approaches a solution, to achieve this effect we have the *learning rate* hyperparameter [4].

The satisfactory error threshold in this type of network is determined by trial and error, making the necessary adjustments to find its ideal characteristics. In the previous tests of the final network model, learning rate adjustments, Split validation and number of epochs were tested, as well as different structures of 2 and 4 layers, finding the lowest training error, MSE of 33 in the configuration.

Once the neural network has been trained, the training files are stored so that they can be used later by another predictionapplication. The MSE and MAE errors are also plotted, shown in Fig. 5, to obtain a clearer idea of the quality of the trained model. A downward trend in MAE and MSE indicates that the metric is improving. This means that the retraining of the model is effective. Erratic or irregular variation indicates that

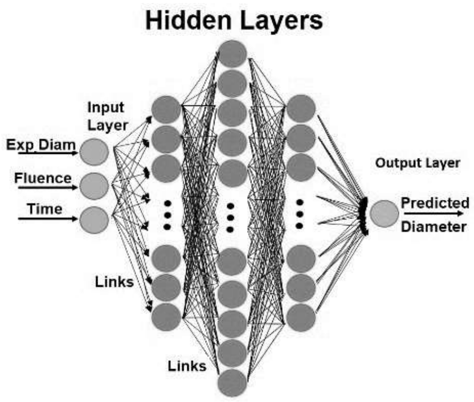

Fig. 4. Representation of the neural network configuration used in this work with its input and output variables.

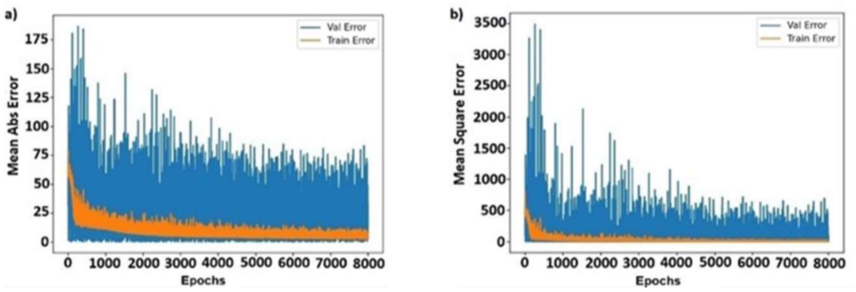

Fig. 5. Representation of the errors obtained, (a) is the MAE and, (b) the MSE of the trained network.

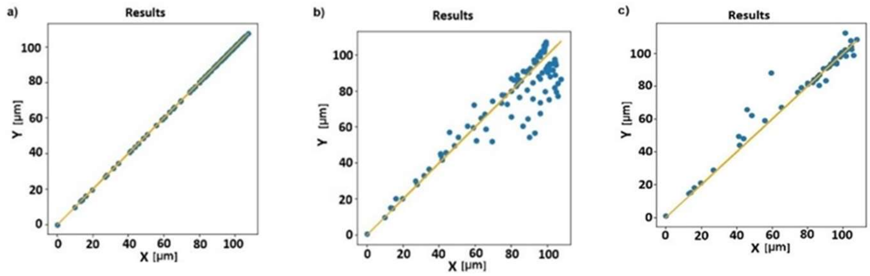

Fig. 6. Distribution of neural network results, (a) Graphed of dataset, (b) Neural network with overfitting, (c) Neural network predictions.

the feedback data is not consistentbetween assessments. Increase the minimum sample size for the quality supervisor. The backpropagation algorithm is based on a recursive procedure to estimate the weights as a function of the response error in each layer [5].

The mean absolute error provides the average of the absolute difference between the model prediction and the target value. The root means square error (MSE) provides the average of the squared difference between the model prediction and the target value. It can be used as a measure of the quality of an estimator. The mean absolute error (MAE) provides the average of the absolute difference between the model prediction and the target value [4].

In some consulted works on deep learning focused on material processing, additional simulation settings, number of times, change of learning rate and hidden layers were made with which a list was made, and the most optimal result was chosen, compared with this work, it was chosen through experimentation and general training data, testing which configuration yielded a better result [2].

5 Results

For the verification of the neural network, sample data obtained from the same training database was used and entered into the prediction application obtaining very small errors and shown in the distribution plot of Fig. 6. Once checking the values, it is possible through this neural network to predict the behavior of the output parameter, through new input parameters.

Each one of the points represents a piece of data, which approximates the training variable and shows the behavior and errors obtained thanks to the neural network. The more adjusted the points are to the line, the better the quality of the predictions obtained.

6 Conclusion

This paper demonstrates the use of neural networks in the analysis of data generated through the experimentation of ultrafast laser pulses, in relation to the effect of the laser fluence, the type of micro processed material, as well as the time spent in each experiment.

In unsupervised learning methods, simulations are performed, and processing results are obtained, before resorting to experimentation, which is sometimes expensive. Much of the work is focused on the preparation and processing of training data takingthe previous experimentation data, as well as the search for the ideal network architecture.

The network shown for this case is simple, although the approach gives us many possibilities for a more robust modeling thanks to convolutional techniques, allowing a better understanding of the study in the transformation of thin metallic filmsby means of ultrashort laser pulses.

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