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Prediction of Physical and Mechanical Properties for Metallic Materials Selection Using Big Data and Artificial Neural Networks

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ABSTRACT In this work, a computer-aided tool is developed to predict relevant physical and mechanical properties that are involved in the selection tasks of metallic materials. The system is based on the use of artificial neural networks supported by big data collection of information about the technological characteristics of thousands of materials. Thus, the volume of data exceeds 43k. The system can access an open online material library (a website where material data are recorded), download the required information, read it, filter it, organise it and move on to the step based on artificial intelligence. An artificial neural network (ANN) is built with thousands of perceptrons, whose topology and connections have been optimised to accelerate the training and predictive capacity of the ANN. After the corresponding training, the system is able to make predictions about the material density and Young's modulus with average confidences greater than 99% and 98%, respectively.

INDEX TERMS Artificial intelligence, big data, material selection, multilayer feedforward networks, neural network, property prediction, software-based web browser control.

LIST OF SYMBOLS AND ABBREVIATIONS

ADAM	Adaptive Moment Estimation
AI	Artificial intelligence
ANN	Artificial Neural Networks
β_n	ADAM algorithm parameter
ϵ	ADAM stability factor
ε	Prediction error of a neural network
η	ADAM step size
f	Error function
g	Gradient of the error function
HTML	HyperText Markup Language
m	ADAM first moment estimate
v	ADAM second moment estimate
w	Weights vector

I. INTRODUCTION

The physical and mechanical properties of a material have a fundamental role in the performance of industrial components. A correct operation depends, to a large extent, on the characteristics of the materials that constitute it as insufficient material properties can cause premature component failure.

In this work, the density and Young's modulus have been chosen as study variables due to their relevance in engineering materials selection tasks. These two characteristics have been profusely applied and investigated, which enables the construction of Ashby diagrams [37], which is an efficient tool in the selection of materials.

Knowing the properties of the materials involved in industrial designs has importance; however, obtaining these data often requires access to a large amount of resources, which are generally not available. A multitude of tests are needed to obtain really significant information, which implies that sufficient time, personnel and facilities must be available at a cost [1]. The process of characterisation of a material may require a battery of tests that requires a considerable amount of time and the investment of vast amounts of resources.

The use of a methodology this is based on trial and error should not be considered since each test implies, as previously indicated, a considerable consumption of resources that are generally scarce. To develop a material from scratch, and

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after a long testing period, realise that it is not valid or does not satisfy the initial specifications, is not possible.

Although extensive libraries of materials with abundant and very detailed information exist, some data needed to perform the work is not always available [2]. Even the most basic information may not be accessible or available, especially when dealing with infrequent, recently developed or the latest technology materials. However, the industry demands that our designs should be taken to their limits, which implies increased use of technological materials [3].

Material libraries can be used to extract trends or general characteristics; however, as the amount of data to be considered increases, the task becomes painful or even impossible [4]. To solve this type of situation, assistance tools can be developed to help the designer [5]. In this way, design loops are reduced and people can concentrate on more creative tasks. The availability of open data becomes increasingly important, which justifies the development of tools to treat information, extract trends or generate new knowledge.

Thousands of material data with adequate tools to extract trends enable the anticipation of the expected properties of a new material without the need for any type of test and limits errors [6]. In this way, research routes can be eliminated before they consume valuable resources that can be exploited in other more productive studies [7].

In this work, the ability of neural networks to extract trends is employed to obtain new information from a material database. The heterogeneity of these data makes traditional database management techniques insufficient, and therefore, the problem must be addressed using newer techniques based on big data.

Big data consists of large and complex data sets, especially from new data sources. Due to the bulkiness of these data sets, they cannot be managed by conventional data processing software [8]. However, these massive volumes of data can be used to address problems that, previously, would not have been possible to solve.

Although the term ''big data'' is relatively new, the action of collecting and storing large amounts of information for further analysis has been performed for many years [9]. The concept gained momentum when the industry analyst Doug Laney articulated the current definition of big data as the three Vs [10]:

- Volume: the amount of data matters. With big data, large volumes of unstructured low-density data are processed. The data can be data of unknown value, such as machining conditions, material properties or manufacturing control measures. For some organisations, tens of terabytes of data are employed; for other companies, even hundreds of petabytes of data are utilised.
- Velocity: the rate at which the data are received, and possibly, to which some action is applied. The higher data-transmission rate is usually conducted directly to memory rather than written to a disc. Some intelligent products work in real time (or practically in real time) and require instantaneous evaluation and action.
- Variety: the various types of data that are available. Conventional data types are structured and can be clearly organised in a relational database. With the rise of big data, data are presented in new types of unstructured data. Unstructured and semi-structured data types, such as text, audio or video, require additional pre-processing to obtain meaning and enable metadata. In addition, big data applications usually cope with sparse information.

Big data enables answers that are more complete to be obtained since more information is available [10]. Having more complete solutions to a problem enables the problem to be addressed with greater guarantees of success and enables resources to be managed a more efficient way [9]. The availability of more complete answers also means greater reliability of information, which implies a completely different approach to addressing problems.

Big data have proven to be a very useful tool in research in materials science and technology. In recent years, many works on this subject have been developed, numerous applications have emerged and important initiatives aimed at serving as a basis for scientists in this field have appeared. Predictive models have been developed based on big data and machine learning [11], and assisted design tools supported by large databases that transform software into an expert system [12] and entities such as the Material Genome Initiative have appeared. The mission of this initiative is to reduce the cost and development time of material discoveries, optimisation and deployment by offering access to large material databases and providing the tools required to ease investigation.

The libraries of materials available on the Internet contain large collections of records that, in general, are incomplete, that is, some properties are not available for a material [13]. The information is actually very sparse, which hinders the ability to obtain valid conclusions using conventional tools [14].

Even though some material libraries are freely accessible [13], in general, downloading large amounts of data is difficult as companies regain their most important information with great zeal.

In this work, the data contained in these libraries have been used to train a system based on artificial intelligence (AI) techniques to extract new information that was not initially available. Note that the quality of the conclusions of this type of methodology is as good as the quality of the data from which the conclusions have been drawn [13]. In this case, the available data have been provided by the material manufacturers themselves and have been certified by standard tests.

Artificial intelligence is the simulation of human intelligence processes by machines, especially computer systems [6]. These processes include learning (acquisition of information and rules for the use of information), reasoning (using the rules to reach approximate or definitive conclusions) and self-correction [15].

Often classified in the cognitive science group, AI uses computational neurobiology (particularly neural networks),

mathematical logic (sub-discipline of mathematics and philosophy) and computer science [16]. AI looks for problem-solving methods with high logic or algorithmic complexity. By extension, AI designates devices or tools by imitating humans in certain implementations of its cognitive functions [15].

The term ''artificial intelligence'' was coined in 1956 during the Dartmouth Conference, where the discipline emerged [17]. Currently, AI is a general term that addresses automation of robotic processes to current robotics. AI has recently gained prominence due to the large volumes of data or to the increase in speed, size and variety of information collected by companies [6]. AI can perform tasks, such as identifying patterns in data more efficiently than humans, which enables users to obtain more information about their data [16].

Since the birth of computer science, a large number of methods and techniques that can be framed within the field of AI have been developed, of which some are more useful than others [18].

Technology enables us to produce materials with an extensive variety of properties; these materials can work very differently depending on the environment and working conditions [6]. This finding implies that a large amount of data are available, and therefore, the situation will become unmanageable using only usual calculation methods. We need tools that can immerse themselves in these data and propose the optimal solution among the options.

A large variety of methods can be framed within the field of artificial intelligence. Among them, artificial neural networks (ANNs) stand out as they have become paradigmatic techniques due to their incredible achievements and unstoppable progress within the field of computing [19].

Artificial neural networks comprise a computational model that is slightly inspired by the behaviour observed in the brain. An artificial neural network consists of a set of units that are referred to as artificial neurons, which are connected to each other to transmit signals. The input information transmits across a neural network, undergoes various operations and produces output values [19].

Frank Rosenblatt defined the perceptron model, which is a supervised learning algorithm of binary classification [20]. This model is a formal neuron with a learning rule that automatically determines synaptic weights to decide whether an input belongs or does not belong to a class. If the problem is linearly separable, a theorem ensures that the rule of the perceptron enables the identification of a separator between the two classes [19].

A set of perceptrons that is organised in several layers has the ability to correctly manage nonlinearly separable problems. These systems rely on error gradient backpropagation models and enable the construction of neuronal models that are as complex as necessary [21].

As systems that are capable of learning, neural networks implement the principle of induction, which is learning by experience [6]. By confronting specific situations,

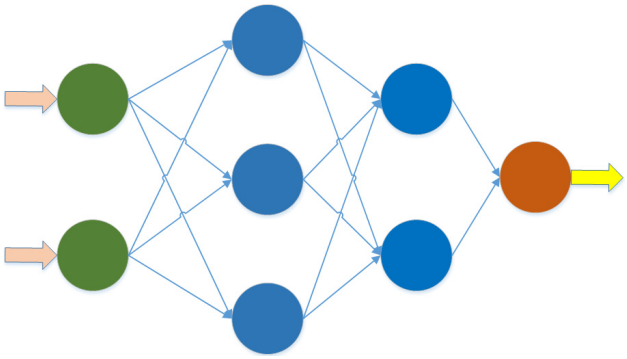

FIGURE 1. Simplified model of a multi-layer artificial neural network.

neural networks infer an integrated decision system whose generic character is a function of the number of learning cases that are encountered and their complexity in relation to the complexity of the problem to be solved [39], [41]. Therefore, complex problems require more training.

Many topological models and neural network architectures exist, among which multi-layer neural networks account for the most prominent networks [21]. Each network attempts to solve some of the problems posed by this type of algorithm: learning process optimisation, reduction of resources for training, and ability to quickly learn certain functions. These systems generally have great plasticity and can be adapted to most types of problems. However, they require large amounts of resources and input data for their training [22].

Fig. 1 shows a simplified model of a multi-layer neural network that is composed by 8 perceptrons, which are organised in 4 layers: 2 perceptrons in the input layer (the layer that receives the data from the exterior), 5 perceptrons in the two hidden layers and 1 perceptron in the output layer (the layer that outputs the processed information).

Table 1 contains some of the most relevant neural network topologies, including a small explanation about its model.

Currently, neural networks are applied in many fields of science and engineering, from control systems [44], [48] to business. Neural networks are a suitable alternative to a large number of methods that are applied in numerous fields. In most cases, even for problems that have been solved by other means and due to different theories, neural networks have identified other more efficient forms of resolution.

Neural networks have a large number of real uses in the industry; they have already identified many commercial applications, as they show better results in the recognition of data patterns or trends than other techniques based on mathematical analysis. Artificial neural networks have proven to be excellent tools for analysing large data sets as, after a training process, they can extract trends that may remain hidden for other conventional systems of information analysis [21].

Our current technological development enables us to produce large amounts of data. However, these data must be processed to obtain reliable and useful information that enables better decisions [6]. Artificial intelligence can help

TABLE 1. Classical neural network topologies [23], [39]–[42].

Topology	Description
Perceptron (P)	A simple mathematical model of a neuron, which simulates the behaviour of a single biological neuron.
Multi-layer feed forward (MLFF)	A model that contains 3 types of layers (input, hidden and output), which propagates the error during the training. These networks can learn any nonlinear function.
Recurrent neural network (RNN)	A MLFF model, whose neurons are trained, not only use information from other neurons but also information from themselves from the previous iteration.
Long/short term memory (LSTM)	A model that attempts to avoid the vanishing/exploding gradient problem of the RNN by introducing gates and an explicitly defined memory cell.
Gated recurrent unit (GRU)	A model similar to LSTM that contains update gates that determines the quantity of information to retain from the last state and the quantity of information to receive from the previous layer.
Auto encoder (AE)	Similar to MLFF. A model that intended to automatically encode information in a compressed way.
Variational AE (VAE)	A model with the same architecture as AE, including some probabilistic cells that avoid non-desired information propagation.
Denoising AE (DAE)	An AE model that is intended to avoid the network to learn details by introducing more noise as input.
Sparse AE (SAE)	An AE model whose aim is to encode information using more space.
Hopfield network (HN)	A fully connected model that always converges to a local minima and whose nodes simultaneously act as input, hidden and output nodes.
Boltzmann machine (BM)	Similar to HN although some neurons are considered input neurons and other neurons remain hidden.
Restricted BM (RBM)	A model similar to BM where some nodes are linked to other nodes; they are mostly grouped.
Deep belief network (DBN)	A model that stacks several RBM or VAE. These networks are able to generate new data.
Deep convolutional network (DCN)	A model that can easily process images or audio and tag them.
Deconvolutional network (DN)	A model that, after training, can produce pictures that are related to a given concept.

designers identify the optimal solution for each task, which can potentially increase the total performance [18].

One of the main tools for the search of the optimum material for an industrial application are Ashby diagrams [37]. This type of scattered plot enables two or more properties of many materials (or classes of materials) to be simultaneously and intuitively visualised. To generate this type of graphic, however, the required data are necessary.

As previously indicated, the libraries of existing free access materials on the internet enable a large amount of data to be available [13]. However, they generally do not authorise users to download complete libraries in a simple way and only allow individual downloading of the data of a single material. In this context, the development of tools that capable of iteratively carrying out this painful task is necessary [14].

These types of websites are protected against the action of bots that can carry out attacks that are aimed at causing the system downfall. Thus, the data download procedure that is developed acts in a similar way to the procedure that would follow a human being, and therefore, building software tools based on web browser control that imitates a user's behaviour is essential [24].

Simplifying, this technique consists of developing code that instructs the web browser that it should behave as if the user had performed daily actions, such as pressing a button, entering a text or downloading a file.

Software-based web browser control consists of the development of code that is aimed at employing browser capabilities: HTML code interpretation, file downloading, permission management, and cookies administration. A web browser provides a wrapper that frees the developed code from the complexity of the operations that are needed to surf the internet [24].

The objective of this work is to determine how artificial neural network technology can be used to exploit a large set of metallic material data [40] to predict its physical and mechanical properties. This work explores the feasibility of training a neural network to ensure that it can predict some physical properties based on the chemical composition of the new materials presented to it.

The purpose of this paper is to establish a framework that establishes the basis for developing the required software and algorithms to determine a broad spectrum of material properties based on their chemical composition. The framework is envisioned as a support tool for the study of materials science.

The main goal of this study is to build an artificial neural network that can receive the material information as input data and make valid predictions. The network topology is optimised to perform this task and enables the collection of output data that is subsequently analysed to calculate the performance of an entire system.

The objectives include the development of software tools that facilitate this work to be carried out (including tools with which the obtained results are analysed) and the procurement of a large set of input data about metallic materials, including their physical properties and chemical composition, and the organisation of big data to ensure that the data were exploitable via the developed algorithms and tools.

The innovation of this work is the use of neural network techniques to build a complete Ashby diagram based on the chemical composition of metals. In addition, the use of artificial neural networks that are trained with a large set of metallic material data to predict their mechanical and physical properties is remarkable.

Neural networks have proven to be very useful in multiple fields to obtain very significant results when combined with reinforced learning techniques using large data sets. However, a limited amount of work applies ANNs to the field of metal science, and most studies that develop procedures aimed at predicting their physical and mechanical properties are based on mathematical or statisticians models instead of artificial intelligence.

The procedure proposed in this work is perfectly scalable and applicable to different types of metals; however, most models can only be applied to a restricted group of

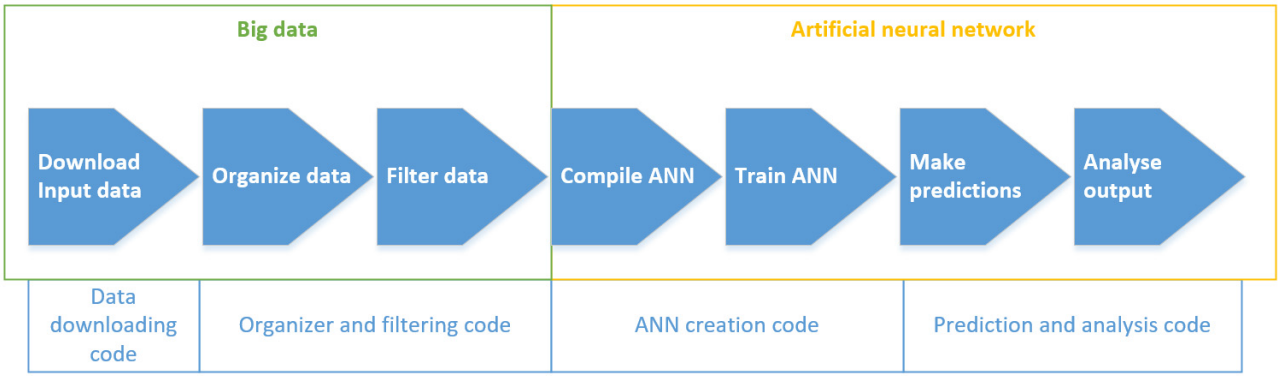

FIGURE 2. Methodology scheme.

materials [49]. The novelty of this methodology is the application of artificial intelligence to the prediction of physical and mechanical properties of metal alloys.

The added value of this methodology consists of the use of artificial intelligence techniques to predict some important properties for the selection of materials in engineering applications. Numerical methodologies only focus on a limited and closed number of material characteristics, while systems based on neural networks can potentially take advantage of all available information to make better decisions.

II. METHODOLOGY

The development of the work has focused on obtaining an artificial neural network that is capable of making adequate predictions about material properties while maintaining a limited average error. Subsequently, the output data, data about the network training process and data about the prediction step are conveniently analysed [16].

A. PRINCIPLES OF THE METHODOLOGY: GENERAL OVERVIEW

Fig. 2 schematically shows the different steps for developing the system. The system has two main stages: the stage related to big data and the collection of input data; and the stage related to the development and use of the artificial neural network (ANN), which also comprises the data analysis. The schematic shows which programming code manages each step.

Matmatch [25] is a well-known open-access materials library that contains information about thousands of different commercial and standard materials. All registered users can freely access the information stored in their databases, whose data are provided by suppliers and manufacturers. A specification sheet that contains all available data can be downloaded for each material. However, the full bulk cannot be downloaded at once, that is, the entire library of materials cannot be downloaded. A software bot that is capable of iteratively downloading (separately) all materials available on the website has been developed.

Once the bot completes its task, therefore, we obtain a collection of thousands of specification sheets about materials that generally contain information about chemical composition, mechanical properties and physical properties. This set of datasheets covers all kinds of materials: metals, ceramics, composites, and polymers.

A second software application runs through all available specification sheets, extracts all contained information (even information that is not relevant for the development of this work), and carries out a small processing and organises it into an easy access matrix. The previously mentioned initial processing consists of the homogenisation of units of measurement and the elimination of non-numerical information (with the exception of the name and the identification, a unique code for each material), which is not susceptible of being exploited.

At this point, we obtain an immense matrix of very sparse data, where each row corresponds to a material and each column represents a property [8]. As previously indicated, some data are not available for certain properties of materials and since the database is very heterogeneous, some properties do not make sense for certain materials [1]. Therefore, this matrix must be filtered to obtain valid input information.

A third code is executed to carry out the filtering of data. Only metallic materials whose chemical composition is defined in more than 90% are considered. During the development of this work, a small amount of the specification sheets did not include the chemical composition of a material or did not correctly detail it. To avoid bias during the training phase, incomplete materials are eliminated [26].

The following chemical elements have been investigated: Al, Fe, Mn, Si, Cu, C, Cr, P, S, Ni, Zn, Mg, Ti, Mo, Pb, Sn, V, N, Nb, W, Sb, As, Bi and Co [27]. The presence of other elements in small quantities does not affect the learning process of the neural network [26]. Note that only metallic materials whose main components are included in this list are considered (i.e., no information related to gold or silver has been considered even if their datasheets have been downloaded).

Fig. 3 graphically shows the results of filtering all available downloaded materials (43575). Materials that are not considered are split into two categories: non-metallic materials (16473) and materials whose chemical definition is

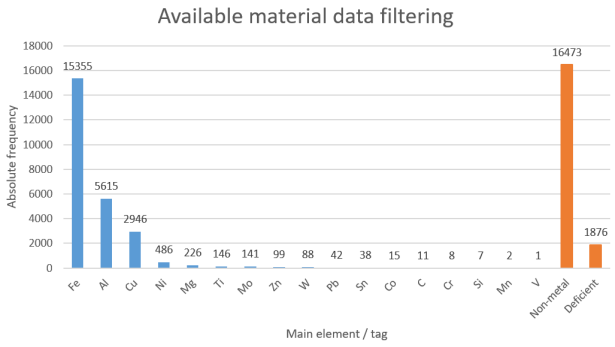

FIGURE 3. Available material data filtering detail.

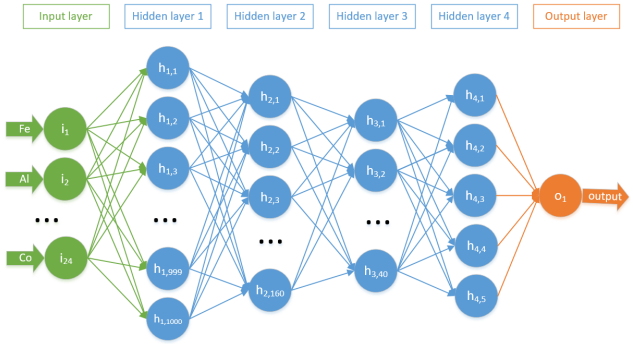

FIGURE 4. Simplified artificial neural network topology.

deficient (1876). The materials that have been effectively employed (25226) are divided according to their main chemical element (17 categories). Materials with a deficient chemical definition include those whose main element is not included in the previously mentioned elements list.

Once the material data are filtered and all information is guaranteed useful and relevant to develop this study, an adequate big data structure is already available. Therefore, the fourth software code is launched to initiate the step based on artificial intelligence [28].

A multilayer feedforward architecture has been chosen and an artificial neural network with a fully connected topology, which consists of an input layer, 4 hidden layers and an output layer, has been defined [22]. The input layer consists of 24 nodes, which correspond to each of the considered chemical elements; the hidden layers are formed by 1000, 160, 40 and 5 perceptrons; and the output layer is formed by a single node. Fig. 4 shows a simplified representation of the neural network topology in this work. The input layer, the hidden layers and the output layer have been differentiated using colours.

This topology is the result of successive optimisation steps to balance its learning capacity and the necessary resources for its training [29]. Note that a complex topology is capable of learning more complex functions than a simple topology but requires additional resources during its training: additional time, calculation capacity and input data [16]. A balance between the network depth and the network width was obtained.

A fully-connected artificial neural network consists of a set of fully connected layers; a fully-connected layer is a layer in which all nodes are connected to all nodes of the next layer [21]. This network is able to learn the function $f : \mathbb{R}^n \rightarrow \mathbb{R}$, where n is the input vector size (in this case, the amount of considered chemical elements is 24) [42].

Hornik [30] showed that the multilayer feedforward architecture provides neural networks with the potential of being universal approximators. Even if a fully connected ANN can represent any function, it may not be able to learn some functions as backpropagation convergence is not guaranteed [22].

Since the network architecture and topology were previously defined, the training phase of the network begins. The available data are randomly divided into two disjoint subsets: training subset and test subset. The first subset comprises 80% of the data, while the second subset contains the remaining 20% of the data. For a data to be used during the learning phase, all input information and expected results are necessary since neural networks are a supervised learning technique.

The network training is subject to the following conditions:

- Calculation of the learning rate for each parameter using Adaptive Moment Estimation (ADAM) where $\beta_1 = 0.9$, $\beta_2 = 0.999$ (algorithm parameters), $\eta = 0.001$ (step size) and $\epsilon = 10^{-8}$ (stability factor) [31].
- Early stopping after 10 iterations without significant changes to avoid overfitting.
- Training stops when a training error of less than 0.001 is reached as it is considered negligible [32].
- Maximum of 100000 training epochs to avoid infinite loops.
- Sigmoid activation function.
- Verbose output to analyse the training process.

Once the neural network has been trained using the corresponding subset of data, predictions can be made using the information from the test subset. In this way, metrics that enable us to measure the performance of the system can be extracted. Several statistical parameters are calculated by comparing the output estimation of the neural network with the real value; these parameters are employed to describe the performance of the network.

B. SOFTWARE AND TOOLS

As previously indicated, multiple software codes have been developed to carry out each of the tasks of this work (refer to Fig. 2). These codes have been developed entirely in Python 3.7 language, although multiple libraries and non-standard modules have been used to simplify some stages of the project. This language has been chosen as Python is a high-level, multi-platform and multi-paradigm programming language with dynamic typing that has great popularity among developers [33], especially, among those who develop software related to artificial intelligence [34].

Some external modules have been employed, such as Selenium (library that enables control of the web browser by using code), BeatifulSoup (library that facilitates working

with HTML files), SciPy (library that contains numerous scientific, mathematical and statistics functions), NumPy (library that enables easy management of large amounts of data and large matrices and numbers), MatPlot (library that eases the production of plots, figures and graphics) [33] and TensorFlow with Keras (high-level library that contains a vast amount of functions and procedures related to artificial intelligence, especially artificial neural networks) [34].

This system comprises more than 9000 lines of code distributed in 11 files that manage different operations.

C. MATERIAL INPUT DATA ACQUISITION FOR FURTHER EVALUATION

As previously indicated, information about materials has been downloaded from an online library via a code that mimics the behaviour of a human user. This task has been achieved by using Gecko Driver 0.24 for Firefox 67.0 and the Selenium module for Python [33]. Gecko Driver and Selenium enables a programmer to ask the web browser to perform actions such as going to a given web page, clicking on an element (i.e., a button or hyperlink) or writing some text in a text-box.

The data downloading code works by the following several steps: identify location of the names of the materials to download, filter to eliminate repeated data, access web record of each material and download the summary data file. This part of the work is extremely slow since it is substantially affected by the speed of the servers where the online library is hosted and the bandwidth of the local network.

After downloading the summary record of each material, we obtain more than 43000 individual files that contain a vast amount of data. These files must be read again to extract their information and organise it in a way that is easily accessible. Once the information is organised in a vast sparse matrix, filtering should be carried out to eliminate data that are not useful or that will not be employed.

These organisation and filtering processes are also carried out via code that was specifically developed for this work.

D. TRAINING AND PREDICTION USING ARTIFICIAL NEURAL NETWORKS

The procedure by which a neural network learns is referred to as training and is mathematically based on the problem of gradient descent [32]. The learning problem of an artificial neural network is the minimisation of the associated error function. This function usually consists of 2 terms: the first term evaluates the adjustment of the network output with respect to the available data (error term) and the second term (regularisation term) is used to avoid overfitting (overfitting is avoided by allowing the training process to eventually stop before overfitting occurs) [35].

The error function entirely depends on the weights associated with each of the perceptrons. This vector of weights with a size equal to the number of neurons (1230) is represented as w and enables us to indicate that $f(w)$ is the error made by the neural network when assigning the weights w to each of the perceptrons that compose it [36]. With this formalisation, the objective of the training is to find the vector $w*$ for which a global minimum of the function f is obtained, which converts the learning problem into an optimisation problem [35].

In this way, a neural network is initialised with some weight vectors (in general, randomly chosen). A new parameter vector is calculated to reduce the error function. This process is repeated until the error has been reduced under a tolerable threshold or when a specific stop condition is satisfied [34].

Since the error function is derivable, the gradient of this function can be defined for each of the optimisation steps (refer to Eq. 1):

$$g_i = \nabla f_i = \nabla f\,(w_i) \tag{1}$$

where w_i is the weight vector for the *ith* optimisation step; f_i is the value of the error in the *ith* step of the iteration; and g_i is the gradient value of the error function in the *ith* step of the iteration [35].

Adaptive moment estimation (ADAM) is an adaptive learning rate method that computes individual learning rates for different parameters. ADAM uses estimations of first and second moments of a gradient to adapt the learning rate for each weight of the neural network [31]. Using this method, in each iteration, the new weights vector is calculated as (refer to Eq. 2):

$$w_{i+1} = w_i - \eta \frac{\hat{m}_{i+1}}{\sqrt{\hat{v}_{i+1}} + \in} \tag{2}$$

where η is the step size (a value that graduates the relevance of the gradient factor), $\in$ is the stability factor of the algorithm (constant) and the bias-corrected first moment estimate $\hat{m}_{i+1}$ and second moment estimate $\hat{v}_{i+1}$ are calculated as follows (refer to Eq. 3 and 4) [31]:

$$\hat{m}_{i+1} = \frac{m_{i+1}}{1 - \beta_1^{i+1}} \tag{3}$$

$$\hat{v}_{i+1} = \frac{v_{i+1}}{1 - \beta_2^{i+1}} \tag{4}$$

where β_1 and β_2 are the algorithm parameters that are set to a value near 1 [31]. m_{i+1} and v_{i+1} are calculated as follows (refer to Eq. 5 and 6):

$$m_{i+1} = \beta_1 m_i + (1 - \beta_1)\, g_{i+1} \tag{5}$$

$$v_{i+1} = \beta_2 v_i + (1 - \beta_2)\, g_{i+1}^2 \tag{6}$$

where m_{i+1} and $v_{i+1}$are the decaying averages of past gradients and past squared gradients, respectively, and are estimates of the first moment (mean) and the second moment (uncentred variance), respectively, of the gradients [31].

The optimisation process and the network training method has been mathematically defined. Once the network has been conveniently trained, predictions can be obtained based on the approximation function learned by the neural network [34].

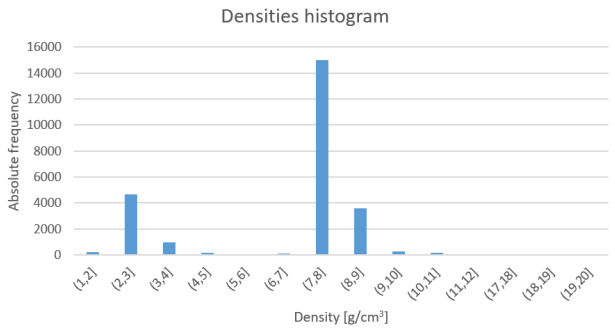

FIGURE 5. Densities histogram.

The prediction deviation is calculated as the absolute value of the relative error of the resulting value (refer to Eq. 7):

$$\varepsilon = \left| \frac{v_{prediction} - v_{real}}{v_{real}} \right| \tag{7}$$

III. RESULTS AND DISCUSSION

Although the training algorithms are randomly initialized, the results (both during training and during prediction) are very stable and converge to the same values with differences below 1% [36]. Only the results of the network that have obtained the best predictive metrics are shown.

Once the neural network is conveniently trained with 80% of the records (training subset), the ANN is requested to make predictions with the remaining 20% of the data (testing subset). In the second step, the network is not given any information about the expected results since this information is information that it must return.

Training and testing using the same dataset is not recommended as bias and overfitting can occur; thus, the obtained results can be fabricated since the performance of the network is not realistic [34].

A. DENSITY TRAINING AND PREDICTION

The neural network is trained with 20180 records of randomly chosen materials, that is, 80% of available materials. For each sample, the ANN is given the percentages of each chemical element (of the 24 elements that are considered) and the density of each material. In this way, the neural network is asked to identify a function that serves as an approximator for the calculation of the density.

Fig. 5 shows a histogram of all densities of the considered materials. The distribution is very irregular as the number of samples exceeds the number of elements. Three remarkable ranges appear: (7, 8], which includes ferrous materials; (2, 3], which includes aluminium alloys; and (8, 9], which includes, among others, brass (Cu + Zn). For these elements, the dataset contains a larger number of samples as they are broadly used materials.

The density of a metal alloy can be well approximated by calculating a weighted average, in which the total density is equal to the sum of the products of the proportions of each element multiplied by its individual density.

TABLE 2. Density training details.

Training samples	20180
Iterations	159
Min. error function value	0.002
Initial error function value	20.976

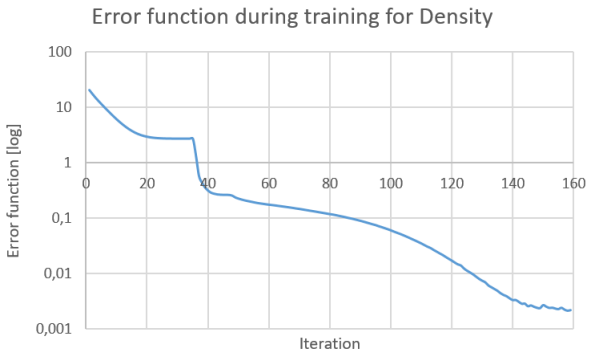

FIGURE 6. Error function during training for the density (log scale).

Note that the ANN is not given the density of each of the individual chemical elements, which is a concept that the neural network must learn supported by the supervised training.

The density-related training process that required 159 iterations ended as no significant improvements occurred during 10 iterations (early stop condition), and a minimum error function value of 0.002 was attained. These data are listed in Table 2. Note that this very low final error function value indicates that the approximation that the network has learned matches the provided data [34].

Fig. 6 shows the evolution (on logarithmic scale) of the error function during the training. Near iteration 35, a very important change in trend occurs; in this step, the ANN learned a significant concept that enabled the error function to be considerably reduced. After iteration 140, the slope of the error function becomes flatter, which indicates that the training process is almost finished (no additional significant improvement).

The neural network is asked to make predictions about the 5046 records contained in the testing subset. For these records, the real density values are known but are not communicated to the ANN as they are retained to calculate some performance metrics.

Table 3 shows some statistical metrics that enable evaluation of the average prediction performance of the network. As shown, the average prediction deviation is 0.448%, and half of the samples are below 0.237% (median). The difference among the average, trimmed mean and median indicates that outliers exist and should be carefully investigated.

Fig. 7 shows the histogram of the errors made in the prediction of the densities of the materials of the testing subset. The samples are accumulated in the first two error ranges, that is, for deviations less than 0.5%. The error is distributed and forms a large peak near 0%, and a long tail of low height appears.

TABLE 3. Density prediction error testing details.

Test samples	5046
Average	0.448%
Std. Dev.	0.855%
Median	0.237%
Maximum	15.157%
Minimum	0.000%
Trimmed mean (±5%)	0.352%
Quartile 1	0.171%
Quartile 2	0.237%
Quartile 3	0.341%

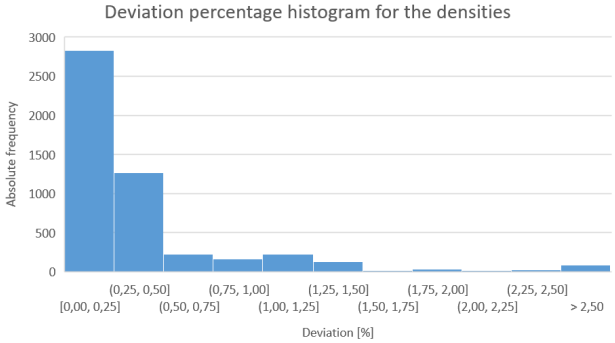

FIGURE 7. Prediction deviation histogram for the density.

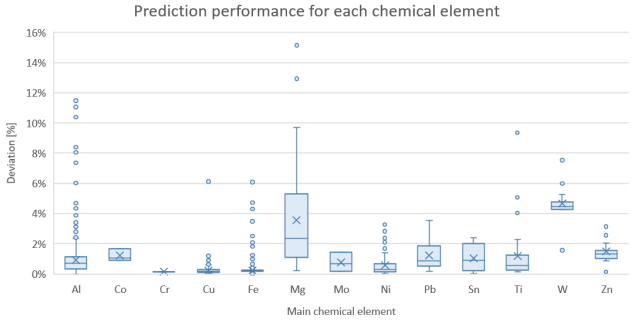

FIGURE 8. Density prediction performance for each chemical element.

Fig. 8 shows the performance of the predictions for each of the main chemical elements of the alloys in the testing subset. Note that the ANN offers substantially worse results for magnesium and tungsten (note that a few samples can be used during the training, which impairs the learning performance). The big box and long whisker related to the magnesium alloys indicates a large predictive variability.

As foreseen by the statistical metrics, Fig. 8 shows some outliers that have been associated with poorly defined materials (note that the quality of the input data is not perfect, although the ANN can address these imperfections). In addition, the neural network encounters problems with some duralumin alloys (they appear as outliers in the chart).

For each main chemical element, Table 4 shows the amount of samples that have been employed during the tests (materials in the testing subset) and the average deviation of the artificial neuronal network when it is making predictions. Significant differences are observed among the elements, although the average error remains bounded. For elements

TABLE 4. Main element related average error.

Main element	Average error [%]	Samples
Al	0.91%	1113
Co	1.22%	3
Cr	0.15%	1
Cu	0.22%	584
Fe	0.23%	3084
Mg	3.55%	48
Mo	0.78%	30
Ni	0.58%	100
Pb	1.23%	9
Sn	1.05%	4
Ti	1.20%	32
W	4.67%	15
Zn	1.48%	23
TOTAL	0.45%	5046

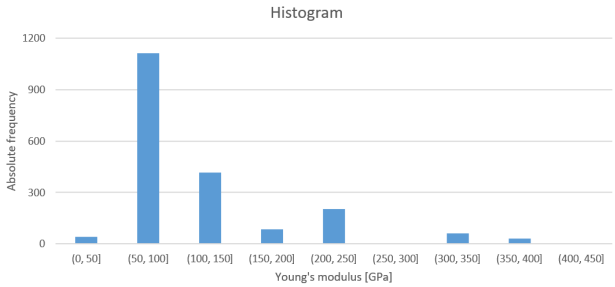

FIGURE 9. Young's modulus histogram.

with a large number of samples (i.e.: aluminium, iron or copper), note that acceptable results are obtained as the ANN successfully learns the density calculation function.

B. YOUNG'S MODULUS TRAINING AND PREDICTION

In this case, the Young's modulus (E) is not available for all materials. Therefore, only materials for which this information is accessible will be considered as these data are necessary in the supervised training phase and the performance estimation phase. Fig. 9 shows the distribution of the Young's modulus among the considered materials. Note that the ranges that contain aluminium alloys (50-100GPa), copper alloys (100-150GPa) and iron alloys (200-250GPa) are much more prominent than the other materials as the dataset contains more samples.

The ANN was trained with 1571 randomly chosen material samples obtained from the samples that can be considered (only 1962 registers contain the Young's modulus value), which is 80% of the data (training subset). For each record, the ANN is given the percentage of each chemical element (among the 24 elements considered) and its corresponding Young's modulus. The neural network is asked to find a function that serves as an approximator for the calculation of the Young's modulus.

The Young's modulus training process required 6693 iterations and ended as no significant improvements were observed during 10 iterations (early stop condition) and a minimum error function value of 548.94 was reached. These data are listed in Table 5.

TABLE 5. Young's modulus training details.

Training samples	1571
Iterations	6693
Min. error function value	548.94
Initial error function value	9123.58

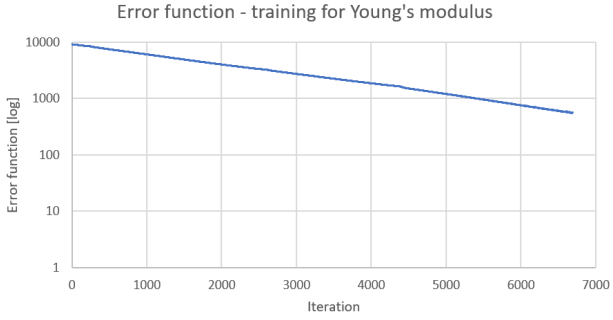

FIGURE 10. Error function during training for the Young's modulus (log scale).

TABLE 6. Young's modulus prediction error testing details.

Testing samples	390
Average	1.561%
Std. Dev.	2.233%
Median	0.667%
Maximum	12.446%
Minimum	0.003%
Trimmed mean (±5%)	1.394%
Quartile 1	0.219%
Quartile 2	0.667%
Quartile 3	1.843%

The final error function value is substantially larger than the density value, which indicates that the training process was not equally performant, and therefore, the predictive capacity of the ANN will be inferior to the previous capacity.

Fig. 10 shows the evolution (on logarithmic scale) of the error function during the training of the neural network for the approximation of the Young's modulus function. A continuous and regular descent that progressively slows until an early stop condition is attained. Although they cannot be observed in the chart, oscillations of some importance occur near the end of the training process, which indicates that the network is not able to continue learning from the available data. Three steps (that can barely be observed due to the chart scale) near iterations 300, 2600 and 4400 are related to significant approximation improvements.

Subsequently, the network is asked to make predictions about the data contained in the testing subset (390 registers). Although we know the real value of the Young's modulus for these samples, this information is not communicated to the network since it will be used to calculate several statistical metrics that can be used to measure the network's performance.

Table 6 contains some statistical metrics that enable us to measure the predictive performance of the neural network. As shown, the average deviation is 1.561% and the error of

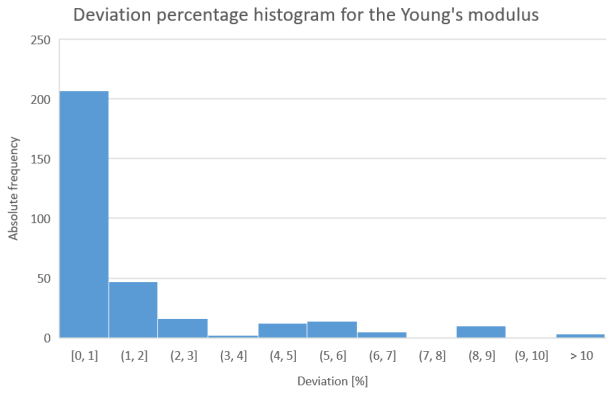

FIGURE 11. Prediction deviation histogram for the Young's modulus.

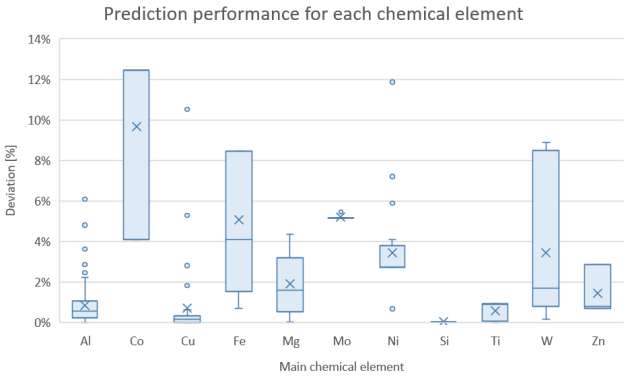

FIGURE 12. Young's modulus prediction performance for each chemical element.

half of the obtained results is less than 0.667%. Note that the average (1.561%), median (0.667%) and trimmed mean (1.394%) are not coincident, which can indicate that some outliers should be carefully investigated.

Fig. 11 shows a histogram in which each sample is related to the range of error in which it is observed. Note the high peak for the range [0, 1] and the long and flat tail. This distribution indicates that the network can make adequate predictions and makes mistakes with some samples.

Fig. 12 shows the performance of the predictions for each of the main chemical elements of the materials in the testing subset. Note that the ANN offers significantly worse results for cobalt and tungsten (note that a few samples are available to use during the training, and therefore, the learning performance is impaired). Fig. 12 also shows some outliers. The big boxes for cobalt, iron and tungsten indicate a large predictive variance.

For each main chemical element, Table 7 shows the number of samples that have been used during the tests (materials in the testing subset) and the average deviation. Significant differences are observed among the groups, although the average error remains bounded. However, for the elements for which a few samples exist, note that the artificial neural network returns worse results. The prediction performance for cobalt and molybdenum alloys is very poor due to the lack of training samples.

TABLE 7. Main element related average error.

Main element	Average error [%]	Samples
Al	0.86%	200
Co	9.67%	3
Cu	0.71%	67
Fe	4.99%	24
Mg	1.92%	10
Mo	5.22%	13
Ni	3.46%	27
Si	0.05%	2
Ti	0.58%	31
W	3.44%	10
Zn	1.46%	3
TOTAL	1.56%	390

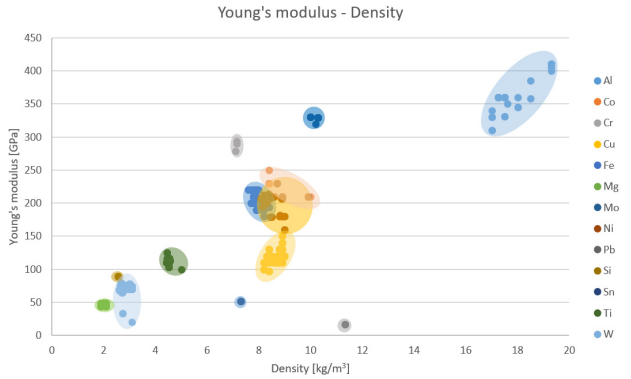

FIGURE 13. Young's modulus vs. density Ashby chart.

C. YOUNG'S MODULUS AND DENSITY ASHBY CHART

An Ashby diagram is a type of scatter plot that enables the relationship between two properties to be established by grouping the points according to a certain criterion [37]. The diagram is a methodological approach to the selection of materials that applies objective principles for the evaluation of the considered properties [38].

Fig. 13 shows an Ashby diagram that relates the Young's moduli of the materials to their respective densities [37]. This Ashby materials selection chart shows clusters of materials that share their main alloy element, which tend to have similar properties.

The diagram has been elaborated using the material data obtained from the predictions made by the artificial neural network. Some elements show substantially greater variability than other elements, which causes a more extensive field. This variability has a negative impact on the performance of the network training since it implies that the function to be learned is more complex.

D. LIMITS OF THE STUDY

The main limitation of this work is the size of the starting data set and the ability of the neural network to learn from this information. As previously indicated, the results of this system improve when the learning process is carried out using a larger input set. However, obtaining large amounts of material data is difficult since the input set it is a very important asset that is not published in an open and easily accessible way. Therefore, a larger initial information corpus can improve the obtained results.

As previously explained, the artificial neural network topology model in this study has some disadvantages (e.g., the results are considerably affected by a reduced initial data set and the local minimums generate substantial attraction) that constitute a limitation of the procedure. Other neural networks architectures can improve the results or reduce the required resources to carry out the training phase.

This study is based on the assumption that the data obtained from the materials library are correct and reliable. Otherwise, the methodology would not change but the obtained results could be affected.

IV. CONCLUSIONS AND FUTURE WORKS

This paper has investigated the feasibility of using artificial neural networks and big data for the prediction of properties of metallic materials whose chemical composition is known. The possibilities of artificial intelligence techniques have been explored based on large data sets. Thus, the major conclusions from this work are presented as follows:

- The artificial neural network technology, as a supervised learning technique, can be employed to exploit large datasets of material information to predict physical and mechanical properties from the chemical composition of different alloys. An ANN can learn to approximate the value of a material property as a function of its chemical constituents.
- An artificial neural network can be trained to predict the density and Young's modulus of a metallic material if its chemical composition is correctly defined. The error of the prediction remains bounded and the average deviation in this work is 0.448% and 1.561%, respectively.
- Supervised-learning methodologies require large training datasets to attain satisfactory predictive performance. The predictive capacity of a neural network improves as the dataset increases as it has more samples to learn from, and therefore, the network is able to learn more precise functions (functions that better approximate the reality of the problem).
- The compiled neural network can adequately approximate the density of a material but requires additional training to attain satisfactory results when it attempts to predict the Young's modulus of an alloy. Note that approximating the density function is theoretically easier with a larger number of samples for training.
- An artificial neural network with multilayer topology can be trained to approximate nonlinear functions related to materials science. Theoretically, a multilayer neural network can learn to approximate any nonlinear function if a sufficient number of samples are provided during the training process and if it has a sufficient number of perceptrons [30].

This work contributes new forms of research for the prediction of other physical or mechanical properties of different types of materials (metals, polymers, ceramics or composites) and enables us to focus future research on materials that are more prominent or for which better results are obtained. In the same way that satisfactory results have been obtained in the prediction of the Young's modulus and the density, the possibility of obtaining useful results for the ultimate stress or the yield stress can be explored.

Artificial neural networks have proven to be a suitable ally for the prediction of physical properties; therefore, they can be employed to describe the elastoplastic behaviour of industrial materials of great relevance without the need to perform expensive and complicated tests of stress-strain. The design of a system that is based on artificial intelligence and capable of completely predicting the stress-strain curve is feasible.

The possibilities of a system whose operation proceeds in the opposite direction to that in this work can also be investigated, that is, we can indicate to the system the properties that we want to achieve, and a system that is based on artificial intelligence can chemically define a material that complies with the indicated requirements.

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