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Neural Network as a Tool for Design of Amorphous Metal Alloys with Desired Elastoplastic Properties

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Abstract: The development and implementation of the methods for designing amorphous metal alloys with desired mechanical properties is one of the most promising areas of modern materials science. Here, the machine learning methods appear to be a suitable complement to empirical methods related to the synthesis and testing of amorphous alloys of various compositions. In the present work, a method is proposed to determine amorphous metal alloys with mechanical properties closest to those required. More than 50,000 amorphous alloys of different compositions have been considered, and the Young's modulus E and the yield strength σ_y have been evaluated for them by the machine learning model trained on the fundamental physical properties of the chemical elements. Statistical treatment of the obtained results reveals that the fundamental physical properties of the chemical element with the largest mass fraction are the most significant factors, whose values correlate with the values of the mechanical properties of the alloys, in which this element is involved. It is shown that the values of the Young's modulus E and the yield strength σ_y are higher for amorphous alloys based on Cr, Fe, Co, Ni, Nb, Mo and W formed by the addition of semimetals (e.g., Be, B, Al, Sn), nonmetals (e.g., Si and P) and lanthanides (e.g., La and Gd) than for alloys of other compositions. Increasing the number of components in alloy from 2 to 7 and changing the mass fraction of chemical elements has no significantly impact on the strength characteristics E and σ_y . Amorphous metal alloys with the most improved mechanical properties have been identified. In particular, such extremely high-strength alloys include $\text{Cr}_{80}\text{B}_{20}$ (among binary), $\text{Mo}_{60}\text{B}_{20}\text{W}_{20}$ (among ternary) and $\text{Cr}_{40}\text{B}_{20}\text{Nb}_{10}\text{Pd}_{10}\text{Ta}_{10}\text{Si}_{10}$ (among multicomponent).



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1. Introduction

Amorphous metal alloys are the promising materials for the automotive, aerospace, energy, electronics and medical technology industries [1–4]. High corrosion resistance, high magnetic permeability, superior mechanical strength, high fracture toughness, high elastic strain limit and high formability are just some of the unique set of properties that make amorphous metal alloys widely applicable [5–7]. Such a combination of properties is directly due to the absence of structural order accompanied by defects, which is typical for crystalline analogues [8–11]. However, despite all the advantages of amorphous metal alloys, their production is complicated by the fact that the formation of a stable disordered structure depends strongly on alloy composition (i.e., number of components, type of added chemical elements) and its preparation protocol (i.e., cooling and compression procedures, initial and final melt temperatures) [12–16].

Amorphous metal alloys are actively studied for more than 80 years, beginning, in particular, with the works of Kramer [17,18]. One of the first methods of practical formation of alloys with amorphous structure was based on the so-called electrodeposition process. Later, in the 60's of the 20th century, the first works related with formation of amorphous metal films by rapid cooling of the corresponding melts were appeared [19,20]. As it turned out later, amorphization of metallic melts of almost any composition is possible

if extremely fast cooling is used. The next stage in the development of the amorphous alloy formation methodology concerned the consideration of alloys in eutectics, where it was found that bulk amorphous samples of more than 1 mm thickness can be formed [21]. Further attention in this area focuses on some aspects. Namely, the mechanical properties of bulk amorphous metal alloys are strongly dependent on alloy composition and chemical purity of raw material. The strength properties of amorphous alloys can be significantly reduced due to the presence of impurities. Moreover, bulk amorphous metal alloys are inherently fragile. Therefore, in the early 2000's, studies were aimed to improve the alloy hardening methods as well as to determine the relationship between the key mechanical properties of amorphous metal alloys, which include the Young's modulus E , the yield strength σ_y and the strength σ_f [22,23]. It has been shown that the relationship between the hardness H (by Vickers method), the strength σ_f , the Young's modulus E and the yield strength σ_y of amorphous metal alloys is close to linear and can be reproduced, for example, by Tabor's relation $H = K\sigma_y$, by Johnson's model $H = \sigma_y(a + b \ln[cE/\sigma_y])$ and by relation $\sigma_f = dE^{1/2}$ (here, K , a , b , c and d are constants) [24–26]. These studies found that amorphous metal alloys with large values of E and σ_y are characterized by high hardness H and strength σ_f .

The synthesis of amorphous metal alloy with desired mechanical properties may require listing various combinations of compositions followed by mechanical testing. This makes the process of synthesizing new alloys extremely difficult and significantly increases the costs. Furthermore, methods of computer design seem to be a suitable support for empirical methods at the stage of determining amorphous metal alloys with desired mechanical properties [27,28]. In recent decades, rapid development of information technologies as well as automation of data collection and storage processes have contributed to the accumulation and systematization of information about the physical and mechanical properties of bulk amorphous metal alloys glasses [29–32]. The methods of machine learning operate with large arrays of the data and allow us to determine the relationship between composition and properties of alloys both already known and not previously known [33–36]. For example, Xiong and co-authors have been developed a machine learning model that can predict the glass-forming ability and elastic moduli of bulk metallic glasses based on the fundamental atomic properties, chemical and physical properties obtained from experiments or density functional theory simulations [37]. These results find the importance of individual chemical element properties and macroscopic properties in determining the strength characteristics of amorphous alloys. The results obtained by Khakurel et al. established that the average concentration of valence electrons, the atomic radius and the melting temperature are the key properties, which are correlated with the Young's modulus of compositionally complex alloys [38]. The results of this work can also be extended to amorphous metal alloys, as it is confirmed in Refs. [39,40]. In addition, as it was found in Ref. [41] using a machine learning model, the Young's modulus of metal alloys under normal conditions correlates with the yield strength and with the glass transition temperature. In this case, the specificity of "chemical formula" of alloy, which is determined by the molar mass and the number of components, is not as important as is usually expected. Johnson and Samwer have found that the mechanical properties (elastic constants, compressive yield strength, elastic strain limit) of 30 bulk metallic glasses as functions of the scaled temperature T_R/T_g obey the universal law $\propto a - b(T_R/T_g)^{2/3}$, where a and b are the constants, T_R is the room temperature, T_g is the glass transition temperature [42]. The results of this work systematize existing knowledge about the mechanical properties of amorphous alloys. An artificial neural network has created by Jeon and co-authors for designing Fe-based amorphous metal alloys with the desired crystallization temperature and glass transition temperature [43]. Thus, all these studies show that the machine learning methods are suitable tool to find new amorphous alloys with required physical and mechanical properties. Despite the significant number of such studies, little attention has been paid to the development of methods for determining previously unknown amorphous alloys with the desired mechanical properties.

The present work proposes a new method for determining amorphous metal alloys of arbitrary composition based on a large set of empirical data. The originality of this method is that it is based on a machine learning model capable of predicting the Young's modulus and the yield strength of amorphous alloys taking into account the fundamental properties of each chemical element that forms the alloys. It is quite significant that the obtained results lead to new knowledge, which will contribute to the determination of amorphous metal alloys that maximally satisfy the required mechanical properties.

2. Method for Determining the Mechanical Properties of Amorphous Metal Alloys

2.1. General Strategy of the Method

The developed method for determining amorphous metal alloys is based on a machine learning model, which is an artificial neural network of direct propagation. The main advantage of this method is the possibility to calculate the Young's modulus E and the yield strength σ_y both for known amorphous metal alloys and for alloys that are yet to be synthesized. The developed method makes it possible to determine E and σ_y of alloys, whose number of components varies in the range from 2 to 7. Note that such the number of components is ordinary for the majority of known metal alloys. In addition, the proposed method can be adapted to identify alloys with large number of components at the presence of appropriate data for neural network training. The composition and mass fraction of chemical elements in the generated alloys are the control parameters, which allow us to construct a diverse set of compounds.

The general strategy for determining amorphous metal alloys implemented in this work consists of four main stages [see Figure 1]:

- *Stage I.* This stage includes the process of data collection and systematization of information about the properties of multicomponent amorphous metal alloys based on Al, Au, Ca, Co, Cu, Fe, La, Hf, Mg, Ni, Pd, Pt, Sc, Ti, W, Zr, etc., as well as information about the properties of the other additional chemical elements involved in the formation of these alloys. Among these properties are the atomic mass m_a , the covalent radius r_c , the ionization energy E_i and the electronegativity χ , which characterize the nature of the chemical element [see Table 1]. This choice is due to the following reasons. First, these parameters most clearly define the possible physical and chemical bonds between the elements, which can either promote or inhibit the formation of an amorphous structure. For example, according to the empirical rule proposed by Inoue et al. in the early 1990's [44], the difference in atomic sizes must be greater than 12% for good amorphization of a liquid. Secondly, most of the intrinsic properties of chemical elements (especially of the same type) are correlated. In addition, the thermal conductivity λ , the specific heat capacity C_s , the density ρ , the melting temperature T_m and the boiling temperature T_b of chemical elements at normal conditions are used. The atomic number Z and the mass fraction m_f of each chemical element in the alloy are used to characterize the alloy composition. The Young's modulus E and the yield strength σ_y are also applied, whose values are known for the considered amorphous alloys. The values of all the listed physical properties are taken from the database *ITPhyMS* (Information technologies in physical materials science) [45] and the database *Materials Project* [46] as well as from Refs. [36,47–50] [see Supplementary data of the present work]. These properties are characterized by different physical dimensions and by different ranges of values. Therefore, the properties are calibrated so that their values vary in the range [0; 1]. The calibration is done according to the rule

$$\text{Property}' = \frac{\text{Property} - \text{Value}_{\min}}{\text{Value}_{\max} - \text{Value}_{\min}}, \quad (1)$$

where “Value_{min}” and “Value_{max}” are the smallest and largest known values of the “Property”. Moreover, all these listed properties correlate with the mechanical properties of materials. For example, Xiong et al. have shown that the accuracy of predicting

the mechanical properties of amorphous metal alloys is improved when the quantities m_a , Z , r_c , ρ , λ , T_m and T_b are considered in a machine learning model [37]. In addition, the results obtained by Wang based on the analysis of a large set of empirical data for amorphous alloys allow one to establish the existence of correlation between elastic moduli (i.e., Young's modulus, shear modulus, bulk modulus), microstructural features, rheological properties, the glass transition temperature, the melting temperature and the boson peak [47,48].

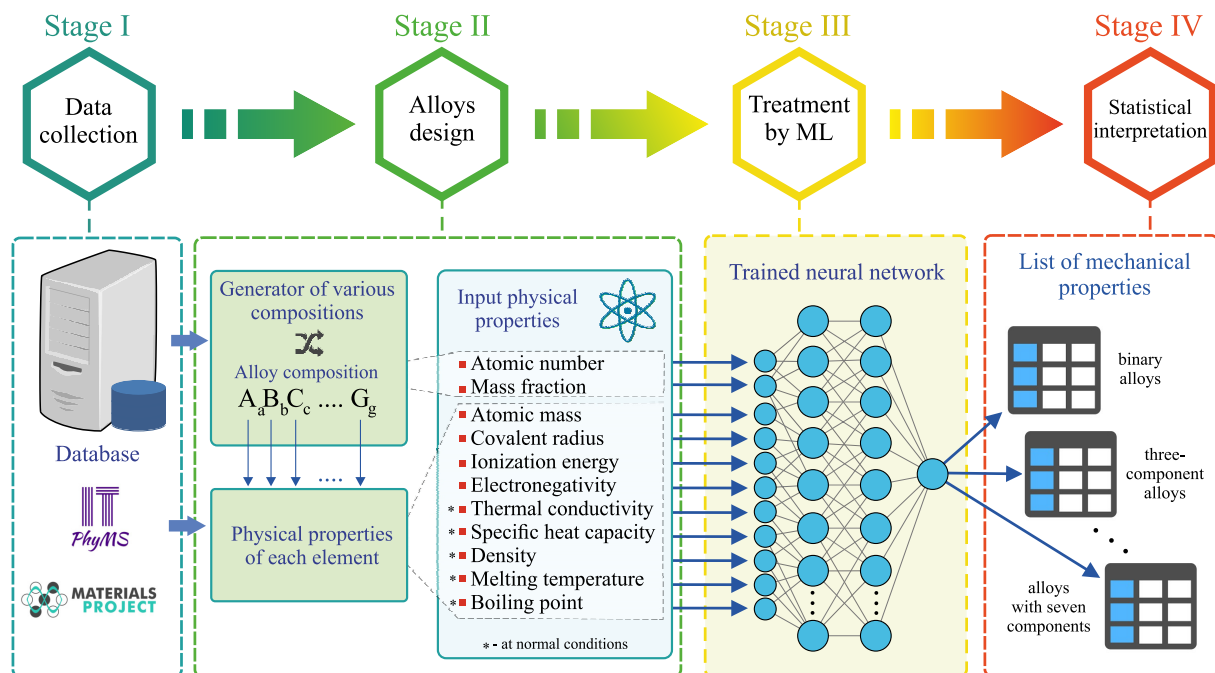


Figure 1. Four-stage scheme of the method for determining amorphous metal alloys and calculating their mechanical properties.

- **Stage II.** Alloys with different compositions are generated. Taking into account the number of possible components, combinations of all chemical elements and their mass fraction, up to 10^{18} different compositions can be determined simultaneously. When obtaining alloys, those chemical elements are selected that are included on the alloys in the training dataset. In the present work, 32 chemical elements were used including transition metals (Fe, Co, Ni, Cu, etc.), semimetals (B, Al, Sn, etc.), lanthanides (La, Gd, Er, etc.) and alkali and alkaline earth metals (Li, Be, Mg, Ca, etc.). A list of all the considered chemical elements is given on Table S1 in Supplementary data. The mass fraction of the chemical elements in a generated alloy is also set randomly so that the total mass fraction of all chemical elements is equal to 100%. A set of physical properties is created for each chemical element [see Table 1].
- **Stage III.** Information about the alloy composition and the physical properties of all the chemical elements is processed by the pre-trained neural network. This neural network evaluates the Young's modulus E and the yield strength σ_y for all generated alloys. The training procedure of the neural network is discussed in more details in the subsection "Machine learning model: structure and training".
- **Stage IV.** Statistical interpretation of machine learning results is performed.

Thus, the proposed method makes it possible to perform a complete cycle of alloy design and determine its mechanical properties: from obtaining the correct alloy composition to calculating the correct values of E and σ_y .

Table 1. Physical properties of chemical elements used as input parameters in the artificial neural network.

Property	Symbol	Unit
Atomic number	Z	—
Mass fraction of elements	m_f	%
Atomic mass	m_a	a.e.m.
Covalent radius	r_c	pm
Ionization energy	E_i	eV
Electronegativity	χ	—
Thermal conductivity	λ	W/(m·K)
Specific heat capacity	C_s	J/(g·K)
Density	ρ	g/cm ³
Melting temperature	T_m	K
Boiling temperature	T_b	K

2.2. Machine Learning Model: Structure and Training

The machine learning model is the four-layer artificial neural network. The first layer has 77 input neurons for the values of 11 physical properties for all chemical elements of the obtained alloy (7 input neurons are allocated to each property because the maximal number of components in the alloy is also seven). If the number of components in the alloy is less than 7, then the remaining neurons are unused. The next two layers are hidden. The first hidden layer consists of 80 neurons, while the second hidden layer has 10 neurons. Note that the number of neurons in the hidden layers is optional. The neural network produces close results with 80 to 100 neurons in the first hidden layer and with 10 to 80 neurons in the second hidden layer. The fourth layer consists of one neuron that determines the Young's modulus E or the yield strength σ_y . It is important to note that two separate independent neural networks with the same structure are used to calculate the values of E and σ_y .

Calculation of the values of all neurons is carried out by expression [51]:

$$n_i^{(k)} = f \left(\sum_{j=1}^{N_{k-1}} w_{ij}^{(k-1)} n_j^{(k-1)} + b_i^{(k)} \right). \quad (2)$$

Here, $n_i^{(k)}$ is the value of the i th neuron in the k th layer ($k = 2, 3, 4$); $w_{ij}^{(k-1)}$ is the value of the $(k-1)$ th layer weight going from a neuron with index j to a neuron with index i from the k th layer; $b_i^{(k)}$ is the bias weight acting on a neuron with index i ; N_{k-1} is the number of neurons in the $(k-1)$ th layer. The sigmoid $f(x) = 1/(1 + \exp[-x])$ is applied as the activation function [52].

The neural network is trained using the backpropagation algorithm [53,54]. The values of the weight coefficients are adjusted as follows:

$$w_{ij}^{(k), new} = w_{ij}^{(k)} - \gamma \frac{\partial \xi}{\partial w_{ij}^{(k)}}, \quad (3)$$

where ξ is the squared error between the output neuron and the desired value of the mechanical property; γ is the training rate. In the present work, the training rate is $\gamma = 0.3$, which is optimal for the created neural network. At the training rate $\gamma = 0.3$, the machine learning model gives the best result for E and σ_y with the lower MRE at the relatively small number of training cycles [see insets on Figures 2a,b]. The original dataset is divided into training and validation subsets in proportion 80:20. The training subset consists of amorphous metal alloys based on Al, Au, Ca, Co, Cu, Fe, La, Hf, etc. with different compositions, for which the values of E and σ_y are known [36,47–50]. The physical properties of the chemical elements of these alloys are also used in the training procedure [see Supplementary Data]. To verify the correctness of the machine learning results, the

validation subset is applied, which includes amorphous alloys that were not included on the training subset. The criterion to stop the training procedure is the minimal error between the results of the output neuron and the required values from the validation subset.

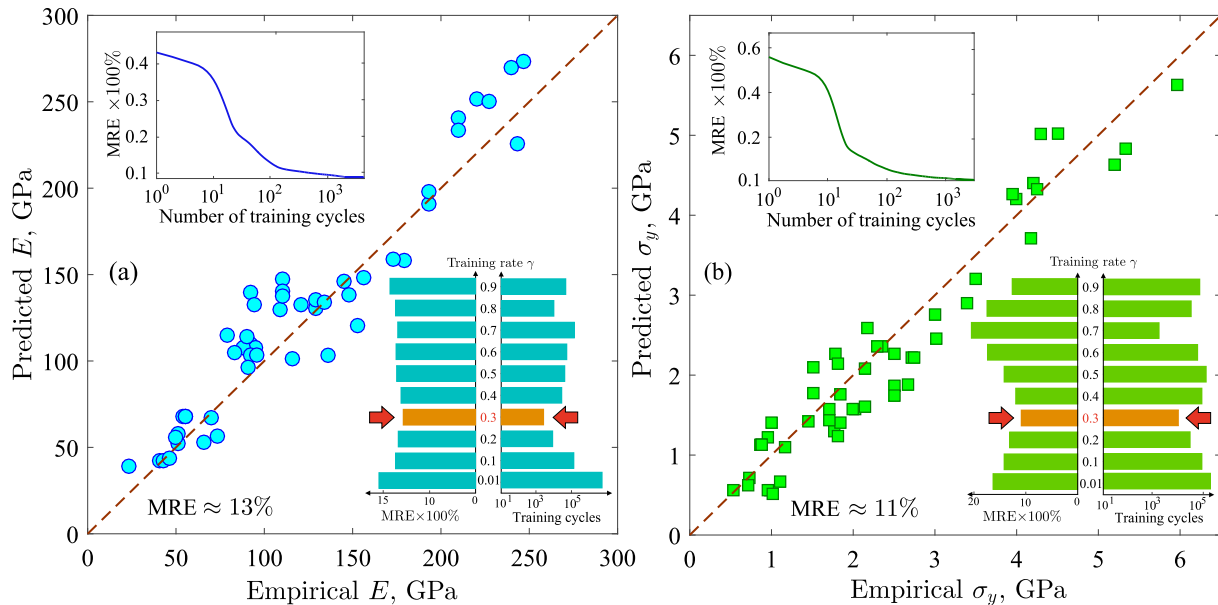


Figure 2. (a) Plot of the predicted Young's modulus E versus the empirical E . (b) Plot of the predicted yield strength σ_y versus the empirical σ_y . Top insets: mean relative error as function of the number of training cycles for E and σ_y . Bottom insets: dependence of the mean relative error and the training cycles on the training rate γ , from which the optimal value of γ (indicated by the red arrows) was determined.

2.3. Validation of the Machine Learning Model

Typically, RMSRE (Root Mean Squared Relative Error), RMSE (Root Mean Square Error), RRMSE (Relative Root Mean Square Error), MSE (Mean Square Error), MAE (Mean Absolute Error) or MRE (Mean Relative Error) are used as indicators for measuring accuracy of results [55–59]. In the present work, it was important to use an indicator that does not depend on units of physical quantities. At the same time, this indicator must be easy to estimate. Therefore, we chose the MRE, which is calculated by expression:

$$\text{MRE} = \frac{1}{N} \sum_{i=1}^N \frac{|\mathcal{M}_{\text{ANN}} - \mathcal{M}_{\text{req}}|}{\mathcal{M}_{\text{req}}} \times 100\%. \quad (4)$$

Here, $\mathcal{M} = \{E \text{ or } \sigma_y\}$ denotes the mechanical property; $\mathcal{M}_{\text{ANN}}$ is the result of the neural network; $\mathcal{M}_{\text{req}}$ is the required value of the mechanical property; N is the number of items in the validation subset. We find that the MRE is $\sim 13\%$ for the Young's modulus E and $\sim 11\%$ for the yield strength σ_y . This relatively low MRE indicates a correlation between the predicted and empirical values of the mechanical properties that is also confirmed by the results presented in Figure 2a,b. Moreover, the values of the MRE are stable. This is confirmed by the computed loss functions [see insets on Figure 2a,b], which reach a plateau after 3×10^3 training cycles. Thus, the results of the machine learning model are reliable and predictable.

3. Properties Importance Scores

The analysis of the importance scores shows that all the considered physical properties (λ , T_b , χ , ρ , C_s , T_m , E_i , r_c and m_a) are necessary for the correct evaluation of the Young's modulus E and the yield strength σ_y by the machine learning model. As can be seen from Figure 3a, in the case of the Young's modulus E , the importance scores of the properties λ ,

T_b , C_s , T_m and m_a are similar (MRE~45%), and these physical properties can be recognized as significant factors. The lowest importance scores are observed for the density ρ and for the properties characterizing the chemical nature of the atoms: the ionization energy E_i (MRE~75%), the electronegativity χ (MRE~61%) and the covalent radius r_c (MRE~60%). These properties have less impact on the result of the machine learning model. Furthermore, considering all the properties reduces the error to MRE~13%. The importance scores of the properties in the case of the yield strength σ_y differ significantly from the Young's modulus E [see Figure 3b]. The main factors affecting the yield strength σ_y are the thermal conductivity λ (MRE~22%) and the covalent radius r_c (MRE~23%). MRE for other parameters is above 28%. Together, these properties lead to the best result, where the error is MRE~11%.

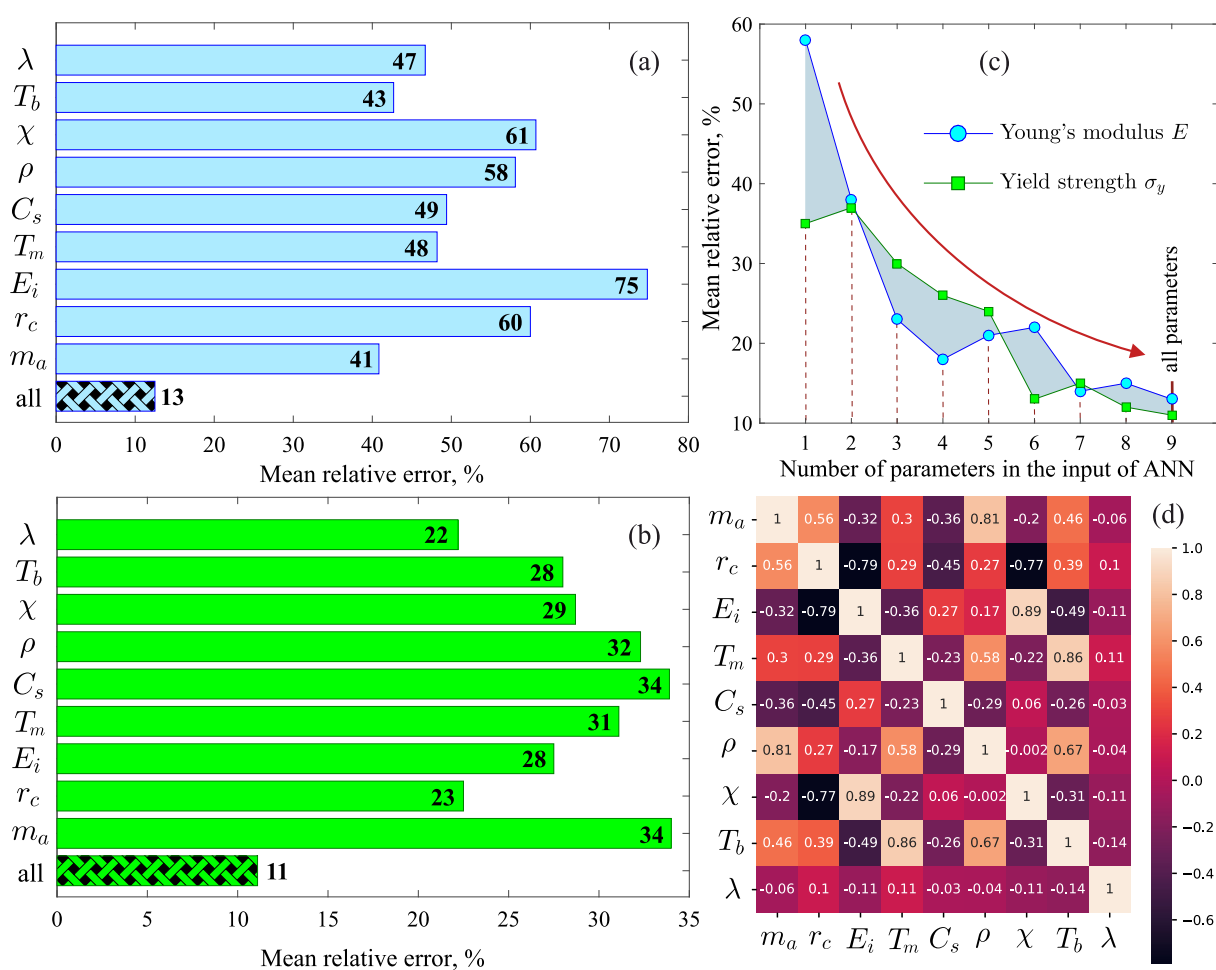


Figure 3. Importance scores for each physical property: (a) in the case of the Young's modulus and (b) in the case of the yield strength. (c) Mean relative error as a function of the number of parameters in the artificial neural network input. (d) Pearson correlation heat map for the considered physical properties.

Thus, the formation of the machine learning models for the Young's modulus E and the yield strength σ_y using a single physical property (λ , or T_b , or χ , or ρ , or C_s , or T_m , ...) produces an error that is much larger than the error when these machine learning models are formed with the entire set of physical properties. Mathematically, such the situation is possible when the correlation between the parameter E (or σ_y) and some individual physical property appears indirectly (not explicitly). In turn, this means that it is not possible to obtain analytical expressions relating a mechanical property with any parameter of the set (λ , T_b , χ , ρ , C_s , T_m , E_i , r_c and m_a) and correctly reproducing the results for an arbitrary metal alloy. The methodology of artificial neural networks used in this study makes it possible to obtain a correspondence between the Young's modulus E (or the yield strength

σ_y) and the whole set of the considered physical properties; and this correspondence is reproduced not by an analytical expression, but by the internal structure of the formed neural network. In fact, this feature of this methodology is an advantage when dealing with a fairly large set of parameters.

An additional evaluation of the accuracy of the machine learning model was performed by computing the MRE for different numbers of physical properties in the input of the neural network. Figure 3c shows that when adding properties in the order of ρ , T_m , T_b , λ , C_s , m_a , r_c , χ and E_i the MRE decreases from $\sim 58\%$ to $\sim 13\%$ for E and from $\sim 33\%$ to $\sim 11\%$ for σ_y . A rapid decrease in the error is observed when the temperatures T_m and T_b as well as the quantities E_i and χ have been added, which may be due to their multicollinearity. Figure 3d shows that the Pearson correlation coefficients for the considered properties take both positive and negative values in the range from -1 to 1 [60]. For example, the positive correlation between the temperatures T_m and T_b is due to the fact that an increase in the melting temperature leads to an increase in the boiling temperature [61]. An increase in the atomic mass m_a of the alloy components usually leads to an increase in the density ρ , which leads to a positive correlation between m_a and ρ [62,63]. The presence of the pronounced negative correlation between the pairs r_c , E_i and r_c , χ is due to the fact that a decrease in the covalent radius r_c leads to an increase E_i and χ by increasing the electron density in the atom [64,65].

4. Statistical Interpretation of the Results

In the present study, 50,000 different amorphous metal alloys were obtained by the proposed method. All alloys were sorted according to the atomic number Z of the basic chemical element and the number of components in the alloy. Using the trained machine learning model, the values of E and σ_y were calculated for each alloy. Furthermore, the average value of the mechanical property was found for each X -based alloy consisting n components (where $n = 2, 3, \dots, 7$). Here, X denotes a chemical element, the mass fraction of which in the alloy is greater than that of other elements. For example, Al-based binary alloys $\text{Al}_{90}\text{Fe}_{10}$, $\text{Al}_{80}\text{Cu}_{20}$, $\text{Al}_{60}\text{Ni}_{40}$, etc. were selected and the average values of E and σ_y were determined for all these alloys. Similar calculations were performed for alloys based on other metals with different number of components. Furthermore, the dependence of the average values of E and σ_y on the atomic number Z of the basic chemical element has been determined.

In the statistical interpretation, the results reveal that E and σ_y depend mainly on the properties of the chemical element with the largest mass fraction. As seen in Figure 4, changing the number of components in an alloy has no significant effect on the values of E and σ_y . In the array of 50,000 different alloys obtained by the machine learning model, some alloys with the highest Young's modulus E and the yield strength σ_y were selected [see Table 2]. The results show that these alloys are mainly based on Ti, Cr, Fe, Co, Ni, Zr, Nb, Mo, Pd, Ta and W. For example, these are $\text{Mo}_{60}\text{B}_{20}\text{W}_{20}$, $\text{Co}_{40}\text{B}_{20}\text{Be}_{20}\text{Al}_{20}$, $\text{Cr}_{40}\text{B}_{20}\text{Nb}_{10}\text{Pd}_{10}\text{Ta}_{10}\text{Si}_{10}$ and $\text{Cr}_{30}\text{Mo}_{20}\text{W}_{20}\text{Pd}_{10}\text{Gd}_{10}\text{B}_{10}$ alloys for which the mechanical properties are $E > 300$ GPa and $\sigma_y > 5.0$ GPa. It is important to note that the results for alloys of these compositions were not previously known, although alloys of some related compositions have been studied. Therefore, for example, for $\text{W}_{46}\text{Ru}_{37}\text{B}_{17}$, $\text{Co}_{43}\text{B}_{31.5}\text{Fe}_{20}\text{Ta}_{5.5}$ and $\text{Co}_{60}\text{B}_{35}\text{Ta}_5$ it was experimentally established that $E > 250$ GPa and $\sigma_y > 5.0$ GPa [41,50]. Obtained results reveal that the alloys based on Cr, Mo and W from the group VI-B of the Periodic Table of the Elements have improved mechanical properties. Such the metals as Cr, Mo and W are refractory and have very high hardness [66–68]. Furthermore, their significant presence in an alloy improves its strength. Note that this fact is also known in metallurgy, where these metals are widely used to increase the hardness of steel alloys, to increase wear resistance and to form wear-resistant coatings (e.g., alloys Cr-Co, Cr-Fe, Mo-Fe, Mo-Cr-Fe, W-Fe, W-Ni-Co) [69,70]. The machine learning model predicts improved mechanical properties in the case of alloys based on Ti, Cr, Fe, Co, Ni, Zr, Nb, Mo, etc. when these alloys are doped with other metals (e.g., Be, B, Hf), nonmetals (e.g., Si, P) and lanthanides (e.g., La, Gd).

The mechanical properties of alloys based on Al, Mg, Ca, Cu, Zn, Ag, Au, Hf, lanthanides, etc. are inferior to those of the alloys based on Ti, Cr, Fe, Co, etc. It should be noted that the relatively high values of E and σ_y purely for B and Si are due to statistical error, since B-based and Si-based alloys were not used in the training stage of the machine learning model. However, alloys containing B and Si were considered.

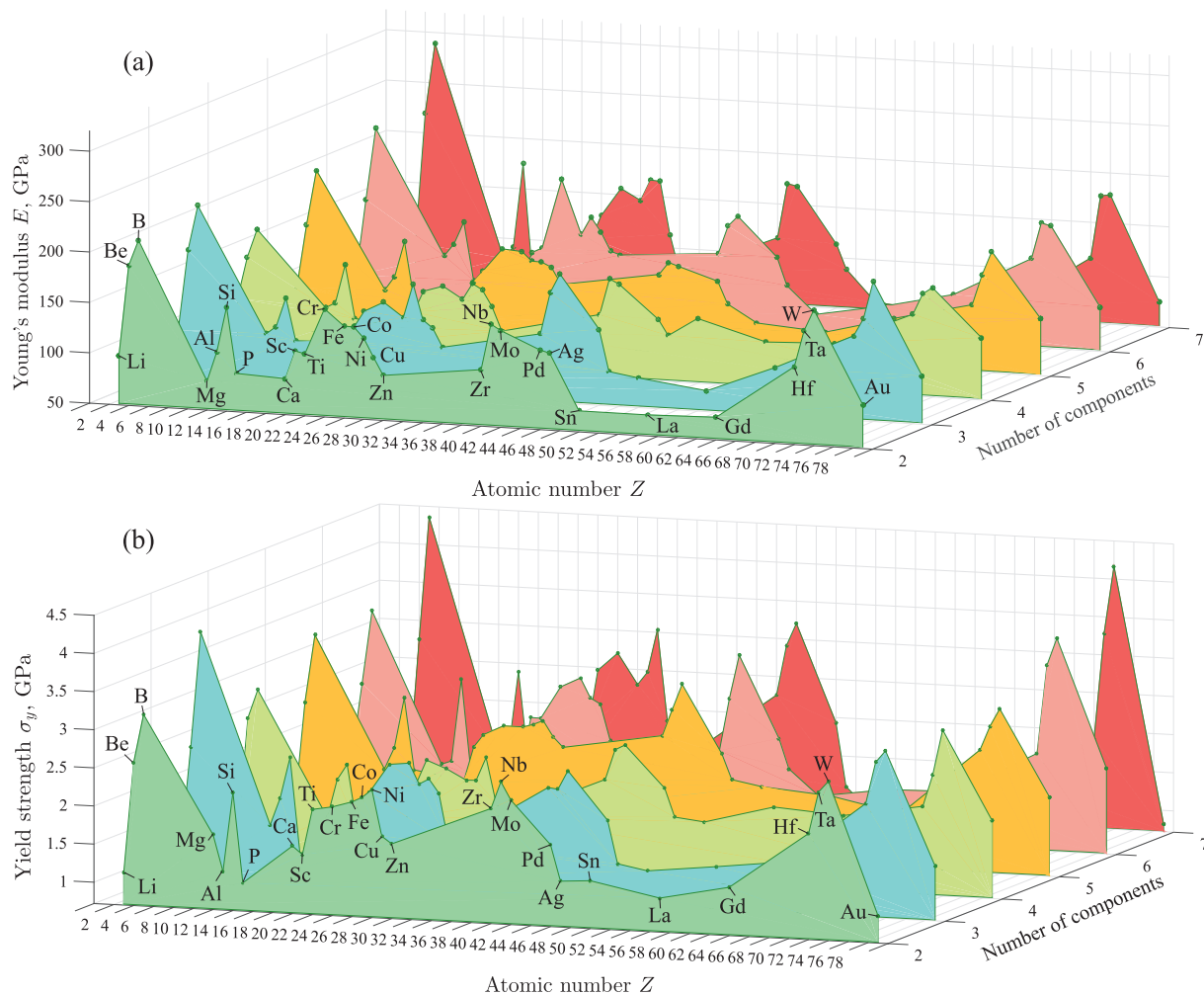


Figure 4. 3D plot of the dependence of the mechanical properties on the atomic number Z of the basic chemical element in the alloy and on its number of components: (a) for the Young's modulus E and (b) for the yield strength σ_y .

In Table 3, we list 10 binary and ternary amorphous metal alloys selected from 50,000 alloys considered in this study. By simple comparison one can reveal that the predicted E is mainly correlated with the mechanical properties of chemical element with the highest mass fraction. For example, for amorphous $\text{Cr}_{80}\text{B}_{20}$, we find $E \approx 305$ GPa, while the Young's modulus of pure crystalline Cr is $E \approx 279$ GPa. In the case of amorphous $\text{W}_{40}\text{Mo}_{40}\text{B}_{20}$, we have $E \approx 318$ GPa, while E is ~ 410 GPa for pure crystalline W. The mechanical properties can vary depending on the concentration of the doped chemical elements and on the class to which these elements belong (metals, nonmetals, lanthanides, etc.). For example, the predicted Young's modulus for $\text{Ni}_{40}\text{Cr}_{40}\text{Co}_{20}$ is $E \approx 58$ GPa. At the same time, the presence of Zr and Si in the Ni-based alloy doubles the Young's modulus E (i.e., one has $E \approx 108$ GPa for $\text{Ni}_{40}\text{Zr}_{40}\text{Si}_{20}$). For $\text{Ni}_{40}\text{Mo}_{40}\text{W}_{20}$, the machine learning model predicts $E \approx 183$ GPa, where the refractory metals Mo and W are included [see Table 3]. The doping with refractory metals, nonmetals and lanthanides (e.g., B, Si, Gd, La) makes it possible to increase the strength of these alloys, which is actively used in modern metallurgy to produce heat-resistant alloys [71,72]. This simple quantitative analysis confirms that the properly selected

composition and physical properties of the main chemical elements are most important in determining the alloys that best match the required mechanical properties.

Table 2. Young's modulus E and yield strength σ_y predicted by machine learning model for different amorphous metal alloys. Here, the average accuracy is $\sim 88\%$.

Number of Components	Alloy	E , GPa	Alloy	σ_y , GPa
2	Cr ₈₀ B ₂₀	305	Pd ₆₀ B ₄₀	5.13
	W ₆₀ Hf ₄₀	271	W ₆₀ Hf ₄₀	5.04
3	Mo ₆₀ B ₂₀ W ₂₀	319	Mo ₆₀ B ₂₀ Si ₂₀	5.35
	Nb ₄₀ Hf ₄₀ B ₂₀	289	Ni ₆₀ B ₂₀ Sc ₂₀	5.17
	Ni ₆₀ B ₂₀ W ₂₀	280	Pd ₆₀ B ₂₀ P ₂₀	4.31
4	Ag ₄₀ B ₂₀ Sc ₂₀ Ta ₂₀	302	Co ₄₀ B ₂₀ Be ₂₀ Al ₂₀	5.27
	Zr ₄₀ Ni ₂₀ B ₂₀ Be ₂₀	285	Nb ₄₀ W ₂₀ La ₂₀ B ₂₀	4.88
	Cr ₄₀ B ₂₀ Zr ₂₀ Hf ₂₀	271	Ti ₄₀ W ₂₀ Pd ₂₀ B ₂₀	4.70
5	Ti ₃₀ Fe ₃₀ B ₂₀ Sn ₁₀ Be ₁₀	296	Co ₄₀ B ₃₀ Ag ₁₀ Gd ₁₀ Si ₁₀	5.54
	Pd ₄₀ B ₂₀ Si ₂₀ P ₁₀ Hf ₁₀	289	Fe ₅₀ B ₂₀ Mo ₁₀ Ta ₁₀ Ag ₁₀	5.39
6	Cr ₄₀ B ₂₀ Nb ₁₀ Pd ₁₀ Ta ₁₀ Si ₁₀	310	Cr ₃₀ Mo ₂₀ W ₂₀ Pd ₁₀ Gd ₁₀ B ₁₀	5.62
	Pd ₄₀ Be ₂₀ Mo ₁₀ Ti ₁₀ B ₁₀ Fe ₁₀	306	Mo ₄₀ W ₂₀ Pd ₁₀ Gd ₁₀ B ₁₀ Cr ₁₀	5.53
	W ₃₀ B ₂₀ Au ₂₀ Be ₁₀ Nb ₁₀ Ag ₁₀	296	Ta ₂₀ Nb ₂₀ Al ₂₀ Au ₂₀ B ₁₀ W ₁₀	5.06
7	W ₂₀ Co ₂₀ Nb ₂₀ Ag ₁₀ B ₁₀ Be ₁₀ Mg ₁₀	284	W ₂₀ B ₂₀ Ag ₂₀ Nb ₁₀ Si ₁₀ Co ₁₀ Pd ₁₀	5.24
	Cr ₂₀ Ag ₂₀ Ti ₂₀ B ₁₀ Gd ₁₀ Be ₁₀ Mg ₁₀	234	Cr ₂₀ Fe ₂₀ W ₂₀ Ca ₁₀ B ₁₀ Sn ₁₀ Be ₁₀	3.78

Table 3. Young's modulus E predicted by machine learning model for binary and ternary amorphous metal alloys. Here, the average accuracy is $\sim 87\%$.

Alloy	E , GPa	Alloy	E , GPa
Cr ₈₀ B ₂₀	305	Cu ₈₀ Mg ₂₀	60
W ₄₀ Mo ₄₀ B ₂₀	318	Cu ₆₀ Mo ₄₀	154
Ni ₄₀ Cr ₄₀ Co ₂₀	58	W ₄₀ Ag ₄₀ B ₂₀	234
Ni ₄₀ Zr ₄₀ Si ₂₀	108	Cr ₄₀ B ₄₀ Gd ₂₀	217
Ni ₄₀ Mo ₄₀ W ₂₀	183	Cr ₄₀ Nb ₄₀ La ₂₀	196

5. Conclusions

In the present study, the machine learning model was applied to predict the Young's modulus E and the yield strength σ_y of amorphous metal alloys with different compositions. More than 50,000 different alloys were determined as well as E and σ_y were evaluated for each of them. It was found that the artificial neural network trained on the basis of information about the atomic number of a chemical element, its atomic mass, covalent radius, ionization energy, electronegativity, thermal conductivity, specific heat capacity, density, melting temperature and boiling temperature allows us to correctly determine of E and σ_y of amorphous metal alloys consisting of 2 to 7 components and containing chemical elements with atomic numbers from $Z = 3$ to $Z = 79$. Here, the mean relative error is $\sim (12 \pm 1)\%$ which is a good accuracy for the direct propagation multilayer neural network. The results of the statistical treatment made it possible to determine the chemical elements with the largest mass fraction, whose presence in the alloy leads to a significant increase in the strength of alloys. These chemical elements are B, Cr, Fe, Co, Ni, Nb, Mo, Pd and W. At the same time, the quantities E and σ_y show a weak dependence on the number of components in alloy. Thus, the most significant factors in the synthesis of alloys with the desired mechanical properties are the properly selected composition and the physical properties of the basic chemical element of the alloy.

Supplementary Materials: The physical properties of the chemical elements used in the machine learning model can be found in Supplementary data and in Github. The following supporting information can be downloaded at: <https://www.mdpi.com/article/10.3390/met13040812/s1>, Table S1: Physical properties of chemical elements used in machine learning model

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