**Significance of Artificial Neural Network Analytical Models in Materials Performance Prediction**

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# Abstract

In materials science, performance prediction of materials plays an important role in improving the quality of materials as well as preventing serious damage to environment and threat to public safety. Traditional regression analysis models in materials science are still not perfect, limited to capture nonlinearities of data and time-consuming for prediction and have poor ability to handle large amount of data. It makes a strong demand on data analysis of materials data with the help of computer science method. In recent years, artificial neural network (ANN) is increasingly performing as a strong bridge between materials science and computer science. In this paper, several ANN applications for predicting various properties of different materials in a variety of materials related areas were reviewed. It highlights the significance of ANN in materials related problems and the trend of ANN in context of materials science with some limitations.

Keyword: materials performance prediction, materials design, artificial neural network, backpropagation neural network, radial basis function neural network

# Introduction

Since material service safety is important to be maintained, many researchers devote their time to experimental testing and data analyzing to discover the different factors influencing on materials performance. Traditional mathematical analysis models used in materials science are still not perfect, limited to capture nonlinearities of data and time-consuming for prediction and have poor ability to handle large amount of data. In recent years, an emerging area of materials performance evaluation and prediction by artificial neural network (ANN) was evolved as an efficient way. ANN analysis can produce satisfactory prediction results of materials properties, compared to traditional data analysis [[1](#_ENREF_1)] [[2](#_ENREF_2)].

One hot research target in materials science is to determine the unknown relations among materials properties. ANN can predict the output by exploring arbitrary interactions among the variables and enabling quantitative expression and understanding of very complicated problems [[3](#_ENREF_3)]. Because of its parallel structure and fast learning capacity, it can be used for linear and non-linear data analyses in applications such as pattern recognition, prediction, system identification and control. The main benefit of neural network is its generalization ability, noise tolerance, fault tolerance and prediction ability of unseen test data with savings in cost and time [[4](#_ENREF_4)].

This paper aims to give a hand to materials and computer researchers with a comprehensive view of ANN models implemented in various prediction applications in material science researches. This review will highlight the significance of ANN in materials related areas and the facts that arouse continuous ANN implementation in future materials related problems.

The rest of the contents are arranged as follows. The basic introduction to ANN, discussed with the principal idea of ANN, the simplest ANN model, various activation functions used in ANNs and different classifications of ANN models, is firstly described in Section 2. Section 3 gives the significance of ANN in materials related researches, ranging from simple MLP and BPNN models alone to more complicated ANN models along with other computing methods, and analyzes their advantages and shortcomings. The future trend of ANN application in materials science is pointed out in Section 4.

# Introduction to Artificial Neural Network

## The Principal Idea of Neural Network

ANN is one kind of network model established in mathematical way that is based upon the working principle of biological neurons connected to each other in biological neural network. In ANN, a neuron is an element that receives multiple inputs and generates a single output and is characterized by its weights, bias and activation function. Those neurons are firstly grouped into layers and then those layers are connected to each other, thus forming a network model. The information from the input layer is moved as the input to the hidden layer that will do linear/non-linear processing to produce the final output to output layer. That kind of movement from the input layer to the output layer is known as feed forward propagation. When there is error between the actual output and the expected output at the output layer, the weights and biases of neurons will be updated to reduce the error in backpropagation process. Learning process, called as training, can learn from previous data and iteratively adjust the weight values to reduce error between actual output and desired output. When the actual output is achieved at a satisfactory level, training is stopped and the weighted links between processing units are saved. The final weights and biases after training are used as analytical tools for prediction of unseen input data. Details of the neural network method itself can be found in [[5](#_ENREF_5)] [[6](#_ENREF_6)] [[7](#_ENREF_7)] [[8](#_ENREF_8)].

## The Simplest ANN

Single layer neural network, generally known as perceptron, is the first and simplest neural network model [[5](#_ENREF_5)]. It consists of only one layer which is composed of neurons. Fig 1 demonstrates a single layer perceptron neural network, in which m and n represent the number of input and the number of neuron respectively and xi connected to all neurons in only one layer and yi are not neurons, just input and output signals.



**Fig 1**. The structure of perceptron (single layer) neural network

As all neurons Fig 1 produce their corresponding output, the number of output is the same as the number of neuron (n). The input signals (x1, x2, …, xm) are connected to the neurons of the single layer via their corresponding weights (w11, w12, …, wnm) so that every neuron has the corresponding weight value for each input signal respectively. It can be seen the first neuron, Neuron-1 has weight data (w11, w12, …, w1m) for input signal (x1, x2, …, xm) as well as Neuron-2 also has its corresponding weight data (w21, w22, …, w2m) for the same input signal (x1, x2, …, xm). It goes in the same way for the nth neuron that its weight data will be (wn1, wn2, …, wnm). The input signal X can be expressed in vector form as

**(1)**

and weight data as

**(2)**

where n is the number of neuron and m is the number of input. Any connection between neurons and input of the network can be calculated based on the number of n and m. For example, Fig 1 shows the connection path between the first input (x1) and the second neuron (n2) can be easily seen as w21.



**Fig 2**. The working principle of a neuron

The working principle of an artificial neuron is shown in Fig 2. As it is mainly constituted with two components: sum and activation function, it can be said that an artificial neuron works in two steps. In the first step, all input data in a neuron are multiplied with their respective weight data and those multiplications are summed to pass through the activation function. The second step accepts the sum as the input to the activation function that will produce the output. The netinput to the activation function in first step can be calculated in vector form as follows:

***netinput= WX =******w1\*x1 + w2\*x2 + w3\*x3+……+ wn\*xm* (3)**

The weighted data (weight \* input) are summed and passed as the input to the activation function of the neuron in the second step. The activation function accepts the input and processes it to produce the output.The output of the entire network can also be calculated by passing the summation of multiplication of the input vector and weight vector to the activation function as follows:

***y= (Netout = F(netinput) =F (WX))* (4)**

To improve the performance of neural network, some neurons includes weight data as well as bias data. By adding bias values b, the performance of the neurons is improved by shifting decision boundary of classifiers to left or right. The value of the bias is generally set to 1 and the mathematical model of the neuron with bias value can be expressed as

***Output*n= (5)**

## Activation Function

Since every neuron uses an activation function to generate output from the weighted data and the accuracy of the output is dependent on activation function, it is important to choose the correct activation function for neurons. The widely used activation functions in neural network architecture are shown in Table 1.

**Table 1**. Activation functions mostly used in ANN

|  |  |  |
| --- | --- | --- |
| **Name** | **Formula** | **Range** |
| **Linear** |  |  |
| **Semi-linear** |  |  |
| **Logistic (sigmoidal)** |  |  |
| **Hyperbolic tangent (sigmoidal)** |  |  |
| **Exponential** |  |  |
| **Sinusoidal (sine)** |  |  |
| **Rational (sigmoidal)** |  |  |
| **Step** |  |  |
| **Hard limit (threshold)** |  |  |
| **Modular** |  |  |
| **Signed (signature)** |  |  |
| **ReLu** |  |  |
| **Leaky ReLu** |  |  |
| **Gaussian** |  |  |
| **Softmax** | for i=1,…, J |  |

Among them, the three most widely used activation functions are linear, sigmoid and hard-limit function. Linear function operates no changes in incoming input signals to generate the original output values. Sigmoid non-linear function, also known as logistic function, can be defined as . It can generate the output between 0 and 1for input value range of -∞ and ∞. Hard-limit function gives the output of neuron as 0 if the input is less than 0; otherwise, it gives the output as 1.

## Classification of Neural Network

Different network models can be basically classified due to the architecture of neural networks: network topology, the number of layers, activation function and type of connection.

### From network topology

The classification of neural network defined by network topology includes completely connected and incompletely connected. Completely connected network means that every neuron of each layer is connected to all the neurons of a neighbor layer. In such kind of network, neurons of one layer transmit their output signal as input to the neurons of next layer. One of well-known completely connected neural network is Hopfield network [[9](#_ENREF_9)]. In incompletely connected neural network, neurons of one layer do not connect to all neurons of neighbor layer, just connecting to some of corresponding neurons from the adjacent layer.

### From the number of layers

The simplest neural network has only one layer. The input and output are connected directly with the neurons in a single layer. Neural networks composed of at least two layers are known as multi-layer neural networks. In multi-layer neural networks, the number of neurons of each layer can be same or different. Layers are connected to each other from left to right order. Network architecture can be described as (number of input layer neurons-number of hidden layer neurons-number of output layer neurons); for example, (5-8-1) structure means 5 neurons in input layer, 8 hidden neurons in hidden layer (hereby (5-8-8-1) means two hidden layers with 8 hidden neurons respectively) and 1 neuron in output layer.

### From activation function type

Activation function is important for the performance of ANN. From Table 1, we can see that there are many different kinds of activation function. ANN can be classified by the types of neurons of the network that use activation function: homogeneous network in which activation functions of the neurons in the network are same and heterogeneous network in which the neurons in the network use different activation functions. Weingaertner et al. presented a framework to develop the automatic design of heterogeneous neural networks by using different activation functions in hidden layer neurons of feed forward neural networks [[10](#_ENREF_10)]. Lee et al. compared their proposed heterogeneous neural network with homogeneous neural network composed of the conventional neuron model, achieving improvement in error rate, training speed, and memory capacity [[11](#_ENREF_11)].

### From connection type

ANN can also be classified if it is feed forward (static) or feedback (dynamic) network according to its feeding direction between layers. ANN layers are usually connected in one direction from left to right order, known as feed forward. Layers of neural networks known as static networks are connected in one direction from one layer to another in feed forward way to calculate the output. But some networks are both feed forward and feedback connected. Feedback networks introduce signal loops (extensive feedback) between the neurons of a layer, and/or between the layers of the network in network in both directions, which are powerful and have more complicated structure. One of popular network models with feedback connection are known as recurrent networks (dynamic networks) [[12](#_ENREF_12)]. Fig 3 illustrates a classification of existing neural network models based on two classes of feed forward and feedback neural network in [[13](#_ENREF_13)] and types of ANN in [[14](#_ENREF_14)].



**Fig 3**. Types of ANN Classified by Connection Type

Besides neural network classifications mentioned above, two or more different types of neural networks can be combined for special purpose, known as hybrid neural network. Such kind of neural networks are multilayer neural networks composed of multiple layers with different topologies and a special learning algorithm is needed for hybrid neural networks.

# Significance of Neural Network Applications in Materials Researches

The generic nature of ANN was widely applied in materials related fields, covering mechanical [[15](#_ENREF_15)], hydrological [[16](#_ENREF_16)], atmospheric science [[17](#_ENREF_17)] [[18](#_ENREF_18)], civil engineering [[19](#_ENREF_19)] and etc., for several application areas in which materials failures can occur, including pressurized water reactors [[20](#_ENREF_20)], quenching operation [[21](#_ENREF_21)] , wrought application [[22](#_ENREF_22)], distribution and transmission electric energy lines [[23](#_ENREF_23)], aqueous chloride solution [[24](#_ENREF_24)], nuclear waste disposal [[25](#_ENREF_25)], aerospace and aviation sectors [[26](#_ENREF_26)], steel production lines [[27](#_ENREF_27)], etc. ANN was established for predicting corrosion in different corrosive environments such as atmosphere [[28](#_ENREF_28)], water [[29](#_ENREF_29)], sea [[23](#_ENREF_23)], high temperature [[30](#_ENREF_30)] and so on as well as forecasting materials performance as failure forms of fatigue [[31](#_ENREF_31)], crack [[20](#_ENREF_20)], pitting [[32](#_ENREF_32)], creep [[33](#_ENREF_33)], flow stress [[34](#_ENREF_34)], wear [[35](#_ENREF_35)], elasticity [[36](#_ENREF_36)], toughness and hardness [[37](#_ENREF_37)], hot deformation behavior [[38](#_ENREF_38)] [[1](#_ENREF_1)], yield strength [[39](#_ENREF_39)], ultimate strength [[40](#_ENREF_40)], elongation to fracture [[22](#_ENREF_22)], etc.

Materials on researches were varied due to the intention materials researchers focused on. Several of them were steel [[41](#_ENREF_41)] [[24](#_ENREF_24)], zinc [[42](#_ENREF_42)], aluminum [[43](#_ENREF_43)], copper [[23](#_ENREF_23)], iron and titanium [[44](#_ENREF_44)], magnesium [[45](#_ENREF_45)], other metal alloys [[20](#_ENREF_20)] [[21](#_ENREF_21)] [[25](#_ENREF_25)] [[26](#_ENREF_26)] [[34](#_ENREF_34)] [[46](#_ENREF_46)] [[47](#_ENREF_47)] and so on. The majority of materials related applications are focused on implementing feed forward BPNN. Recent works on other powerful, complicated and efficient neural networks models, such as radial basic function neural network (RBFNN) [[22](#_ENREF_22)], convolutional neural network (CNN) [[48](#_ENREF_48)]and generalized regression neural network (GRNN) [[49](#_ENREF_49)] can also give satisfactory prediction. The dataset for all those ANN modellings were obtained from experiments as well as from some references. In materials science researches, it is important to know the role of variables affecting on material properties and determine which input variable is the most influencing factor on desired output variable. Some input ranking methods, such as change of MSE (COM), fuzzy curves and sensitivity analysis, have been applied to extract knowledge from trained ANN [[50](#_ENREF_50)]. Previous recent works have shown that integration of neural networks with other computing paradigms such as Bayesian framework [[51](#_ENREF_51)], genetic algorithm [[52](#_ENREF_52)] [[2](#_ENREF_2)] [[53](#_ENREF_53)], sensitivity analysis [[54](#_ENREF_54)] [[42](#_ENREF_42)] [[24](#_ENREF_24)] and fuzzy logic[[45](#_ENREF_45)] can effectively be used to make the performance of neural network models more efficient. The development of more than one ANN types (such as linear model (LM) (simplest form of ANN), MLP, radial basis function (RBF) and so on) and hybrid use of different ANN models were also discussed in some researches in literature [[55](#_ENREF_55)] [[56](#_ENREF_56)] [[57](#_ENREF_57)] with their comparison results with experimental results.

Bhadeshia [[58](#_ENREF_58)] reviewed on some weakness of traditional linear regression analysis and why neural network architecture came up to replace linear regression analysis with specific neural network applications in context of materials. We summarize the majority of neural network prediction models exploited in materials related problems for predicting different properties of different materials in general, shown in Table 2. Most of those ANN prediction results were agreed with experimental results. The definitions of the nomenclatures in Table 2 are described in Appendix.

**Table 2**. Neural network predictive models used in materials related problems

|  |  |  |  |  |  |  |  |
| --- | --- | --- | --- | --- | --- | --- | --- |
| Materials | Applied Area | Experimental Environment(that produce data for ANN model) | Input | Activation Function | Output | Predicted/ relevant Property | Neural Network Model |
| steel and zinc[[42](#_ENREF_42)] | industrial applications | atmospheric environment | T, TOW, exposure time, SO2 and Cl- | sigmoid | corrosion depth | chemical | MLP |
| 304 Stainless Steel[[24](#_ENREF_24)] | industrial applications | aqueous chloride solution | T, Cl- and P | sigmoid | time of failure as a result of SCC | mechanical | MLP |
| Al, low carbon steel, copper[[23](#_ENREF_23)] | distribution and transmission electric energy lines | atmospheric environment | environmental parameters(exposure time, T, RH, precipitation, TOW, WV, solar radiation, Cl-, sulfur compounds and dustfall) | linear and sigmoidal tangent, logarithmic | laboratory evaluated atmospheric corrosion rates | chemical | MLP |
| Iron alloy, carbon and alloy steel, grade-2 titanium[[44](#_ENREF_44)] | industrial applications | atmospheric and chemically defined environments | Mo content x, Ni content (14 x), (x + 1), HCl, H2SO4, E, dE (general corrosion DC data on iron-alloy)  compositions (B, C, Cr, Cu, Fe, Mn, Mo, Ni, P, S, Si, Ti, and V), exposure time, log (exposure time) (general corrosion DC data on carbon and alloy steel)  incubation period and the duration of experiments (localized corrosion crevice corrosion on Ti-alloy) | hyperbolic tangent | log(i), Ecorr, icorr, and Rp (general corrosion DC data on iron-alloy)  corrosion rate and log (corrosion rate) (general corrosion DC data on carbon and alloy steel)  Dmax, W, Q, ratio Q/W, O2 consumed, log (Dmax), log (W), log (Q), log (Q/W), and log (O2consumed) (localized corrosion crevice corrosion on Ti-alloy) | chemical | MLP |
| nickel-based alloy 22[[25](#_ENREF_25)] | industrial (nuclear waste disposal) | BSW-12, temperature, pH, chloride concentration, saturated NaCl electrolyte  (chemically defined environments) | T values, sample treatment types: welded or annealed, and exposure time (general corrosion)  sample treatments: welded or annealed, T, pH, Cl-, aging time, types of corrosion: general or localized (localized (service)corrosion)  w and log(w) (localized corrosion) | hyperbolic tangent | corrosion weight loss (general corrosion)  repassivation potential (localized corrosion),  Zr, Zi, abs(Z), and Phase (localized corrosion) | chemical | MLP |
| A357 alloy [[21](#_ENREF_21)] | aerospace, automotive industries | quenching operation | deformation temperature, SR and S | tan sigmoid and log sigmoid, linear | flow stress | mechanical | BPNN |
| Alloy 600[[20](#_ENREF_20)] | pressurized water reactors (PWR), steam generator (SG) tubing and penetration nozzles | PWR environments | T, KI, pH, Conductivity, ECP, YS, B3(OH)3, Li | hyperbolic tan (tanh), linear | CGR | mechanical | BPNN |
| Sn-Ag alloy[[46](#_ENREF_46)] | electronics industry | inhibitor addition  (chemical environment) | the contents of In. Bi, Sb, RE, Sn, Ag, Cu | sigmoid, purelin | tensile strength, shear strength and solidification temperature | mechanical | BPNN |
| Ti-5Al-2Sn-2Zr-4Cr-4Mo alloy[[47](#_ENREF_47)] | industrial applications | elevated temperature  (on Thermechmastor-Z hot simulator) | deformation temperature, equivalent SR, and equivalent S, | sigmoid, linear | flow stress | mechanical | BPNN |
| steel[[41](#_ENREF_41)] | concrete structures and buildings | open atmosphere | time intervals | sigmoid | electrical potential as a factor for steel corrosion | chemical | BPNN |
| dual-phase (DP) steels[[31](#_ENREF_31)] | earthmoving machineries, gas pipelines, chemical industries and defense | corrosive environment | SIF (ΔK), and volume % of martensite content (%M) | gaussian | FCGR (da/dN) | mechanical | BPNN |
| Al7075-T6, Al2024-T315, D16 aluminum alloy,  350 WT steel[[26](#_ENREF_26)] | aerospace and aviation industry | constant amplitude loading  (from other reference) | SIF, stress ratio | gaussian | CGR | mechanical | RBFNN |
| polyphenylene sulfide (PPS) matrix composites [[59](#_ENREF_59)] | tribological application | dry testing conditions and room temperature | material compositions (PPS matrix, Short carbon fiber, TiO2, PTFE, Graphite), Testing conditions (Sliding speed, Applied pressure) | tansig, purelin | tribological characteristic (Coefficient of friction, Specific wear rate) | mechanical | BPNN |
| microalloyed pipeline steels[[60](#_ENREF_60)] | petroleum industry | standard glass cell | chemical compositions (C, Mn, Nb, Ti, N, Mo, Ni, Al, Cu, Cr, V and CEIIW), microstructure consist of diffusion (ferrite/pearlite) and shear (bainite/martensite) transformations, and corrosion cell characteristics (reference electrode, scan rate, T, PO2, PCO2, NaCl, bicarbonate concentration) | hyperbolic sigmoid, linear | Icorr and Ecorr | chemical | BPNN |
| microalloyed API X70 line pipe steels[[37](#_ENREF_37)] | oil and natural gas industries | thermomechanical processing environment | chemical compositions (CEIIW, CEPcm, VTiNb, NbV, CrMoNiCu) and tensile properties (YS, UTS, El) | hyperbolic sigmoid, linear | toughness and hardness | mechanical | BPNN |
| Ni–SiC composite coatings[[61](#_ENREF_61)] | industrial applications | ultrasonic electrodeposition cell | Up, Csic, and Cd | not clearly defined | weight loss | chemical | MLP |
| prestressed, posttensioned concrete (PC)[[62](#_ENREF_62)] | civil and structural engineering applications | accelerated carbonation experiment | SL, W/C, C/FA, C/CA and TA | not clearly defined for BPNN, radial basis function for RBFNN | DC | chemical | BPNN and RBFNN |
| steel reinforced concrete[[19](#_ENREF_19)] | civil engineering applications | Laboratory environment under constant relative concrete humidity conditions | T, ρAC,bar , ρAC,conc, ρDC | not clearly defined | icorr | chemical | MLP |
| mild steel[[63](#_ENREF_63)] | building industry | turning process | *f, v, d* and *a* | gaussian | Ra | mechanical | radial basis function network |
| aluminum alloys[[64](#_ENREF_64)] | aerospace and other fields | atmospheric environment | altitude, annual average temperature, average humidity, annual average sunshine and annual rainfall | not clearly defined | atmospheric corrosion rate | chemical | BPNN |
| structural carbon steel[[65](#_ENREF_65)] | industrial applications | atmospheric environment | T, RH, amount of precipitation, pH, SO2 and exposure time | not clearly defined | atmospheric corrosion weight loss | chemical | MLP |
| AA3004 aluminum alloy[[43](#_ENREF_43)] | can making | hot rolling, cold rolling and annealing processes | the ratio of initial to final thicknesses, reduction, preheating time and temperature, finish rolling temperature and the final annealing temperature | logistic sigmoid | YS, El, UTS, , | mechanical | BPNN |
| steel strip[[66](#_ENREF_66)] | industrial applications | HP hydraulic descaling operation | spray pressure, water flowrate, spray angle and vertical spray height | purelin, tansig | spray impact | mechanical | BPNN |
| aluminium-based, particulate-reinforced metal matrix composites (MMCs) [[67](#_ENREF_67)] | structural applications | stirr casting process | different SiC (µm) particle size ranges | sigmoid | density and tensile strengths | mechanical | MLP |
| IN625 alloy [[34](#_ENREF_34)] | aeronautic, aerospace, marine, petrochemical industries and gas turbine engine components | hot compression test  (from other reference) | T, SR and S | sigmoid (tansig and logsig) | flow stress | mechanical | MLP |
| mild steel [[68](#_ENREF_68)] | chemical and industrial applications | three-compartment glass cell | Hammett constants, dipole moment, HOMO energy, LUMO energy, energy gap, molecular area and volume | sigmoid | corrosion inhibitor efficiency | chemical | MLP |
| sandcrete materials [[36](#_ENREF_36)] | civil engineering projects | uniaxial compression | W/B, MK, B, SP and  UV | logistic sigmoid, hyperbolic tangent | compressive strength, Modulus of Elasticity | mechanical | BPNN |
| structural carbon steel[[28](#_ENREF_28)] | industrial applications | atmospheric environment | T, RH , precipitation, pH, SO2 and exposure time | not clearly defined | corrosion weight loss | chemical | MLP |
| Ti–6Al–4V alloy[[69](#_ENREF_69)] | aerospace, auto- motive and marine industries | turning process | s, t, v | tansig, Purelin | Ra | mechanical | MLP |
| carbon steel manganese [[70](#_ENREF_70)] | oil industry | corrosive environment | time, T and inhibitor concentration of inhibitor | gaussian | Zr and Zi | chemical | RBFNN |

## ANN for Typical Materials Performance Prediction

To predict materials properties is a challenge in materials related fields because it relies on a large number of variables that are in complex nonlinear relation with each other. ANN are empirical models that can elucidate any unknown correlation in physical models and satisfy complex problems in materials [[71](#_ENREF_71)]. Therefore, ANN was given an attention of materials researchers for predicting properties related with mechanical [[21](#_ENREF_21), [27](#_ENREF_27), [40](#_ENREF_40), [72](#_ENREF_72)] [[30](#_ENREF_30)]and tribological and wear [[73](#_ENREF_73)] [[59](#_ENREF_59)] [[59](#_ENREF_59), [73](#_ENREF_73)][[74](#_ENREF_74)]. There were also many published satisfactory ANN predictions dealing with chemical property in corrosion related problems [[23](#_ENREF_23), [25](#_ENREF_25), [44](#_ENREF_44), [75-78](#_ENREF_75)]. Some experimental techniques such as corrosion test, tensile test, theoretical deterministic methods, metallographic corrosion characterization, mechanical testing and AC impedance spectroscopy, etc., were used to acquire the data for ANN training and result verifying.

Regarding to space requirement, it is not possible to describe all ANN applications in details so that some of them will be grouped and reviewed into three different properties.

### Chemical Property

Electrochemical reaction on materials surface by nature is known as corrosion. The atmosphere can cause a big deal in corrosion degradation process of materials. Statistical regression analysis models mostly used for prediction cannot give superb performance because complexity and non-linearity of meterological variables on atmospheric corrosion is apparently high. To observe local atmospheric corrositivity, in the region of São Luis, five Atmospheric Corrosion Stations (ACS) were installed to monitor the local atmospheric corrosivity and three representative metallic specimens of low-carbon steel, copper and aluminum were exposed to the atmosphere for almost two years. According to corrosivity degree measurement of ACS test sites, the corrosion rates and thickness losses of low-carbon steel, copper and aluminum were respectively categorized into three corrosion metrics: generalized corrosion, alveolar corrosion and localized corrosion. A mathematical model based MLP ANN was established by Kenny et al., (2009) [[23](#_ENREF_23)], with linear and sigmoidal tangent transfer function at the first hidden layer and logarithmic transfer functions at the second intermediate layer by using Levenberg–Marquardt backpropagation training algorithm, to analyze corrosion rates of three different matereials. Meterological data of ten specific environmental variables (time of exposure, T, RH, precipitation, TOW, WV, solar radiation, Cl-, sulfur compounds and dustfall) collected were used as the input to train ANN and laboratory evaluated corrosion rates of specimens were used as the output to analyze the atmospheric corrosion rates. The good correlations obtained in the analysis demonstrate ANN performed greatly in estimating the corrosion rate. It supports one major benefit of ANN that ANN performs well in estimating high complexity and nonlinear correlation between input and output parameters. Long-term corrosion prediction could be calculated by Pourbaix equation[[79](#_ENREF_79)] evaluated with parameters derived from ANN analysis for two year period.

To deal with different corrosion metrics of different materials, Kamrunnahar and Urquidi-Macdonald (2009) [[44](#_ENREF_44)] developed more than one multilayer perceptron backpropagation ANN model to predict different kinds of corrosion behavior. Three ANNs were modelled for two general corrosion data on iron-alloy, and carbon and alloy steel, and one localized corrosion data on Ti-alloy. The ANN model developed for grade-2 titanium showed excellent agreement with experimental data and then used for prediction of future maximum pit depth and other variables under similar operating conditions, giving very good agreement results with experiments. In 2010, Kamrunnahar and Urquidi-Macdonald have also done an extended work [[25](#_ENREF_25)] of their previous work [[44](#_ENREF_44)]. But in that work, they emphasized on different corrosion metrics of one material. They established three different neural networks for localized and general corrosion of alloy 22, with the best network structures of 8-5-5-1 for localized cervie corrosion, of 2-100-100-10-4 for localized corrosion, AC impedance data and of 4-5-5-1 for general corrosion study. The aim of both works was to predict corrosion behavior of metal alloys such as metallic glasses, carbon steel, and grade-2 titanium as well as alloy 22. Data from two different sources (publicly available publications, etc. and personal communication) were together brought into ANN models. Both works have shown that ANN prediction results were good agreement with experimental data.

Concerned with electrochemical reaction, Bassam et al., (2008) [[77](#_ENREF_77)] and Colorado-Garrido et al., (2008) [[78](#_ENREF_78)] have also implemented prediction ability of MLP neural networks in the application of electrochemical impedance techniques. Bassam et al., trained a MLP neural network model with 4-5-1 network architecture, Levenberg–Marquardt learning algorithm, hyperbolic tangent sigmoid and linear transfer functions for the determination of different types of corrosion by using electrochemical impedance spectroscopy curves from different inhibitor concentrations. Correlation coefficient of R>0.9905 described good agreement between simulations and theoretical data test. It was expected that the model may also enable the implementation of smart sensors for online quality determination (corrosion type) in pipeline steel. Colorado-Garrido et al., described the application of MLP neural network to electrochemical testing by predicting impedance spectroscopy values, with the same network parameters used in the work of Bassam et al.,. The best network architecture was obtained with 2-5-1 for 5 ppm of inhibitor and 2-2-1 for 25 ppm of inhibitor, and correlation coefficients R value of 0.984 for 5 ppm and 0.994 for 25 ppm described good agreement between simulations and theoretical data test. In this case, the model’s aim was to predict the imaginary impedance based on the real part of the impedance as a function of time to determine the corrosion resistance of the tested material in the solution. By using the same network parameters, the performance results of those two works gave good agreement between actual and predicted data.

,Also, it can be concluded that a good ANN model can progressively be used for future prediction in context of the problem with same nature, from the works of Bassam et al., and Colorado-Garrido et al.

### Mechanical Property

Multivariate nonlinear regression method has been used to represent complicated interaction of flow stress with strain, strain rate and temperature. But the complicated correlation of flow stress with their affecting factors (microstructure and processing parameters) is difficult to be evaluated by any simple constitutive model. To overcome the repeated calculation of regression parameters for new experimental data in simple constitutive model, Yang et al. (2012) [[21](#_ENREF_21)] developed an accurate thermal stress model with strain rate and strain, to solve the problems of quench distortion of parts by ANN with a back propagation learning algorithm. In this model, the author used batch training from two network training types: sequential training and batch training. Batch training of BPNN with the best network structure (3-6-8-1) including two hidden layers provided about 3% error rate between the predicted output and the actual output. According to a strong positive linear correlation relationship between predicted data and experimental data by correlation coefficient calculation, the model was chosen to achieve good network performance for predicting for thermal stress of quenched A357 alloy with a higher precision. In this work, the authors were concerned with training types of ANN so that stability was found in performance of network.

Sasikumar et al., (2008) [[40](#_ENREF_40)] presented a BP neural network, that had the best training result with 66-45-1 network architecture, and AE (Acoustic Emission) amplitude frequency data collected up to 50% of failure loads were used as input to BP neural network for failure load (ultimate strength of unidirectional T-300/914 tensile specimens) prediction. Levenberg-Marquardt algorithm and the linear transfer function were used for establishing ANN. In this work, it can be found that the network could not predict the ultimate loads outside the training range in trained network. At this point, it made incapability of the network because it is necessary to subsequently add the AE data of specimens with extreme error rate that lies beyond the training range into the training set, thereby decreasing the acceptable maximum error rate from 8.37% to 1.22%. Other key parameters such as duration, energy, events and counts were also used along with BP Neural Network for material characterization and structural integrity evaluation for further analysis. From analysis, it was found that amplitude frequency is the most affecting factor in predicting failure load of composite hardware.

The author have done another similar work in [[72](#_ENREF_72)] in which three different BP neural networks were built for predicting failure strength of composite tensile coupons using acoustic emission technique. But up to 30%, 40% and 50% of failure loads were used as input to three neural networks. Three optimal network structures are 66-37-1 constructed with 30% of AE data, 66-22-1 constructed with 40% of AE data and 66-45-1 constructed with 50% of AE data, respectively. All of them applied the same network parameters like learning rate of 0.01, momentum of 0.9, hyperbolic tangent transfer function, and backpropagation training algorithm. However, the comparison of three networks showed that the network trained with more data could provide better performance.

The purpose of both works by Sasikumar et al., was to to reduce the structural degradation of composites. Reducing the proof test load is the only way for structural degradation. By ANN analytical models, the prediction results of tensile strength in both works indicated that proof test can be done on more sophisticated composites at lower loads so that the actual failure load of composite hardware was predicted. But there was same finding from both works that inadequate training data did not produce the optimal prediction.

### Tribological Property

[[77](#_ENREF_77" \o "Bassam, 2008 #443)][[78](#_ENREF_78" \o "Colorado-Garrido, 2008 #446)]Predicting tribological properties of polymer composites friction materials to determine performance potential is a challenge in materials science because the available experimental dataset is relatively small, noisy, complex and highly non-linear, and the process of developing and testing a new composite material on trail-error based experimental method is time-consuming and laborious as well as complex and costly. ANN can make the problem-independent solution to prediction of tribological properties due to its advantage of nonlinearity, adaptive learning, and generalization. Gyurova and Friedrich (2011) [[80](#_ENREF_80" \o "Gyurova, 2011 #718)] established two MLP neural networks for predicting tribological properties (coefficient of friction and specific wear rates) of polyphenylene sulfide (PPS) matrix composites. A new measurement series was performed with thermoplastic matrix composites and preexisting five experimental training datasets collected or expanded throughout a period of three years were used for training and testing the developed network models. Material compositions and testing conditions were used as input parameter to predict the tribological properties. The tansig function and purelin function were used as transfer functions for the hidden layer and the output layer respectively. The best network structures achieved with coefficient of friction and specific wear rate were 7-[3-1]2-1 and 7-[9-3]2-1, respectively. A user-friendly graphical interface was developed for performing network training and prediction and it could easily predict even for unseen input. The network performance was evaluated by a comparison of the MRE (mean relative error) generated after training of the ANN with the different training datasets, thereby improving significantly with the enlarged datasets. The satisfactory ANN predicted results had good correlation with the measured values. The optimized ANN models was also used to analyze the impact of SCF (short carbon fiber), sub-micro TiO2, on the sliding friction and wear properties of PPS composites. It gave the excellent generalization of ANN without performing exhaustive experimental work. When those ANN models were also applied for studying the effect of internal lubricants (Gr and PTFE) in hybrid polymer systems, good correlation existed between actual and predicted output.

Liu et al., (2007) [[73](#_ENREF_73" \o "LiuJie, 2007 #453)] predicted friction coefficient and wear weight loss of carbon-fibre-reinforced polyetheretherketone composite (PEEK-CF30) as a function of *pv* factor and contact temperature by two BP neural network models of which generalization capability was improved by implementing Bayesian regularization in combination with Levenberg–Marquardt learning algorithm. The best network was obtained with (2-7-1) and (2-8-1) architectures and sigmoid and  
pureline transfer function were used for hidden and output layers. In this work, the authors were dealed with data normalization and unnormalization methods so that the importance of each parameter was balanced and the networks were trained smoothly about 33 and 56 cycles. Those well-trained ANNs gave optimized generalization capability such that friction coefficient and wear weight loss were predicted with high accuracy of relative error lower than 10%. From the analysis, it was found that friction coefficient was strongly effected by the value of *pv* factor whereas compact temperature is the strongly influencing factor for wear weight loss.

It was shown that tits makes to be used e and produces the highly accurate prediction results. It can be seen that predicting triobological properties of materials by ANN models reduces excessive experimental work by yielding satisfactory and acceptable results compared to experimental results and ANN performance can also be optimized with other computing technologies, such as bayesian regularisation framework.

## ANN for New Materials Design

The relation among composition, process and properties of new materials design are influenced by many complicated factors. In the context of materials science, ANN performs a great job for prediction and function approximation with respect to materials’ performance, but there are not many ANN applications enough for forecasting materials properties for materials design. Li et al. (2007) [[46](#_ENREF_46)] studied a new route for the designing of lead-free solder that can find out the influence of adding input variables (the contents of In. Bi, Sb, RE, Sn, Ag, Cu) to tensile strength, shear strength and solidification temperature of Sn-Ag alloy by using multilayer BP Neural Network. The best network structure 7-40-40-40-1 with three hidden layers was chosen. Data from one reference came into the ANN for training and testing. The analysis result showed that the error rates between expected output and predicted output was within 5%, but only one of them gave 7% error rate because of less amount of training data, unexact measurement of shear strength and poor-proportionally distributed data. This work also indicated that more accurate prediction results can be obtained with big amount of training data. However, ANN still gave good agreement with given experimental conditions and it was verified for making the feasible estimates of the property of the lead-free solder.

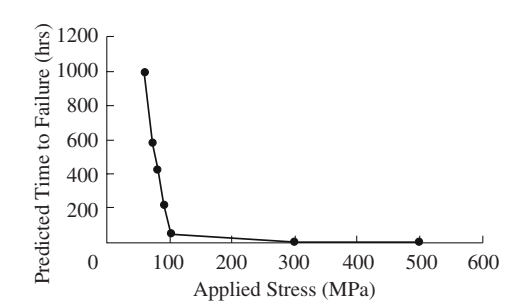
Xie et al., (2018) [[48](#_ENREF_48)] developed a highly accurate prediction model of density functional theory (DFT) calculated properties from Materials Project [[81](#_ENREF_81)], with a database of a diverse set of inorganic crystals ranging from simple metals to complex minerals (including 46744 materials covering 87 elements, 7 lattice systems, and 216 space groups). A crystal graph convolutional neural networks (CGCNN) framework, an innovated universal and interpretable representation of crystalline materials, could directly learn material properties from the connection of atoms in the crystal and discover empirical rules of materials design, that were consistent with the common knowledge for discovering more stable materials. Thus, the search space for high-throughput screening could significantly be reduced by additional information provided by CGCNN for material design. Traditional methods used to represent the arbitrary size of crystal systems as a fixed length vector was well replaced by CGCNN by grabbing the benefit of deep learning. The authors also designed a new convolution function to make learning deeper networks easier, that improved generalization ability of CGCNN as well as prediction performance of different materials properties. Compared to previous statistical learning (SL) framework presented by De Jong et al., [[82](#_ENREF_82)] that implemented multivariate local regression to predict elastic properties on the same dataset, CGCNN provided similar results, but it had advantage of predicting properties by extracting features only from the crystal structure. And when CGCNN model was used for 1585 new crystals that were recently added into Materials Project database, it could also provide a good generalization to materials from potentially different crystal groups. It was a kind of evidence that ANN has good generalization ability. CGCNN could also predict discrete properties as well as the classifications of metal and semiconductor with the same framework by using a softmax activation function for the output layer and a cross entropy cost function.

Most current ANN materials applications highlighted the advantage of feed forward neural networks and ANN performance results were pointed out as being superior or similar in making comparison with experimental results. The authors in [[48](#_ENREF_48)] just brought a great contribution into materials science by implementing the concept of deep learning to mine valuable knowledge from a large dataset to accelerate the design of crystalline materials.

## ANN with Other Computing Paradigms

Integration of neural networks with other computing paradigms, such as Bayesian framework, fuzzy logic, sensitivity analysis and genetic algorithm, can also enhance the performance of ANN. Cai et al., (1999) [[42](#_ENREF_42)] used multilayer perceptron ANN analysis integrated with sensitivity analysis to analyze phenomenon of atmospheric corrosion behavior of steel and zinc. This work investigated a system with environmental variables including temperature (T), time of wetness (TOW), exposure time and concentrations of Sulphur dioxide (SO2) and chloride (Cl-), and found out the complex interactions between those variables and atmospheric corrosion. The database was big enough to be used for this work, including information from corrosion tests, climatological tables and rainfall data from thirty-three countries around the world. But those data were measured by different methods in different sources so that corrosion data might have inherently scattered. According to sensitivity analysis, almost linear relationship between TOW, SO2 (the most affecting input variables on atmospheric corrosion in industrial environment) and atmospheric corrosion of steel and zinc were found at a specified condition. The network structure (5-8-1) with one hidden layer and sigmoid transfer function showed that the ANN results accounted for approximately 70% of the variance seen in the real data sets. Although this work did not consider about other possibly more important parameters on atmospheric corrosion (such as effect of microclimate) for prediction model, it can be seen that ANN could still give more satisfactory results by its fault-tolerance ability than previous linear regression analysis.

To find out the solution to the challenge of predicting the time to failure of 304 stainless steel as a result of SCC (stress corrosion cracking) in aqueous chloride solution, Lajevardi et al., (2009) [[24](#_ENREF_24)] have implemented a similar approach adopted by Cai et al., in which a MLP with backpropagation algorithm was constructed and evaluated using the collection of experimental data associated with the SCC of AISI 304. The data used to train the network was extracted from 24 references. The best network structure was (3-4-4-1) with sigmoid transfer function. In this work, Montecarlo optimization has been used to evaluate the initial set of weight values to reduce the local optima phenomenon. Both of those works have conducted sensitivity analysis to improve the network efficiency by demonstrating the effects of the important variables and showed the effects of the other affecting variables. Sensitivity analysis in Fig 4 showed that among three input parameters (applied stress, temperature and Cl-), applied stress was regarded as the most influencing parameter on time to failure. Those ANN models can account for about 70% and 74 % of the variance of the experimental data, but these two works have some limitations in unseen possible affecting variables, unexplained variances in prediction and data accuracy.



**Fig 4.** Effect of applied stress on time to failure (Cl– = 2100 ppm and a = 130 MPa) [[24](#_ENREF_24)]

Xia et al., (2016) [[45](#_ENREF_45)] used another effective input ranking method called fuzzy curve to rank the importance of input parameters that might have great impact on the output. The authors built two BP neural networks for investigating non-linear correlation and predicting hardness and corrosion rate of magnesium alloy as a function of compositions. ANN prediction results demonstrated that there was an excellent correlation for hardness and although correlation for corrosion rates was lower than hardness, it was still considerably good result because of the inherently chemical activity of Mg and complex interactions between alloy additions. Fuzzy curve analysis was also used in integration with ANN to analyze the impact of each alloying element on the performance of alloy. The sequence of the alloying elements in terms of their ability to improve the performance of Mg alloys was ranked with relatively low alloying level for high hardness as Ca ≥ Zr  Sr Zn Gd whereas fuzzy curves gave complex results for corrosion rate, but the impact of each alloy element on corrosion rate were respectively described. It can be seen that non-linear correlations have been existing between hardness and corrosion rate. However, fuzzy curve analysis could improve the performance of ANN with satisfactory accuracy and the model can be used for corrosion prediction of other existing and future Mg alloys.

ANN is a technology that can learn by examples and then make prediction for new situations. ANN model needs sufficient amount of adequately extensive and representative data to constitute a good training set to solve the problem. Many unnecessary input parameters that do not have a strong interaction with desired output in training data makes an exhausted training and degrades the network performance. In materials science researches, it is critical to know the importance of each input variables affecting on material properties and identify which input variable is the most influencing factor on materials’ properties. By using input ranking methods like sensitivity analysis and fuzzy curve, unimportant input parameters will easily be found out and to be eliminated from the problem and then model will be made simpler and easier to define future possible mechanisms, and the solution will be more fruitful and exact. And modelling ability of ANN can be improved by considering all other possible variables that have stronger impact on output at a given condition and by constructing a more enriched dataset.

The benefit of other computing technologies, such as genetic algorithm and Bayesian framework, can save the defects of ANN model, like overfitting occurred while training the network and uncertainty and instability of ANN, and then the performance of network is significantly improved. That fact was supported by the work of Huang et al., (2018) [[2](#_ENREF_2)] in which the authors have made a comparison of three different approaches to predict flow behavior and find out the optimum hot working processing parameters of 5754 aluminum alloy as a function of deformation parameters. Three forecasting models: strain-compensation Arrhenius (SA), back propagation (BP) ANN and an optimized BPANN model based on genetic algorithm (ANN-GA) were constructed. Their comparison showed that four-layered BPANN model provided more accurate prediction than SA model. But it was found that BPANN model was weak to optimize globally so that local optimum occurred in learning algorithm. This weakness made instability in network performance. BPANN was optimized by genetic algorithm (GA) to form a new model with network structure (3-10-8-1) that produced high accuracy and stability (Correlation Coefficient R=0.9999 and Average Absolute Relative Error ARRE=0.0232–1.0485) within the whole deformation range by calculating the fitness values of each individual in GA by the predictive error norm of the neural network. Therefore, ANN-GA model was found as the most efficient and accurate model among three models because genetic algorithm (GA) can remove the uncertainty of ANN, improve its stability and accuracy by searching for the optimal weight and threshold for ANN at the same time.

In [[66](#_ENREF_66)], Kermanpur et al., (2007) used steel strip data set from the hot strip mills of Mobarakeh Steel Complex to construct a novel analytical predictive framework, named analytical–artificial neural network (AANN) model to estimate the spray impact from spray angle, spray pressure, vertical spray height and water flowrate. The predictive model was coupled with Bayesian regularization that can reduce the overfitting problem of Levenberg–Marquardt ANN learning algorithm and improve the network prediction ability for unseen data. The combined network can be used as a proper tool to evaluate the efficiency of a high pressure (HP) hydraulic descaling operation using flat spray nozzles in terms of achieving the highest spray impact under any process condition. With an optimal network structure of one input layer with four input variables, two hidden layers and one output layer with one output variable, a maximum amount of output (spray impact) was obtained. The prediction result showed good agreement with correlation coefficient R2 of 0.992. In this work, sensitivity analysis was also carried out in which input parameter spray angle resulted in the highest influence on spray impact is followed by the spray height. The authors were also progressively using their current AANN model to predict the effect of all input parameters on the spray overlap.

In recent works, we can see that there are many successful ANN applications in materials related problems. Herein, the hybrid system, the joint implementation of other computing methodologies in which ANN plays in a major role, can make more satisfactory improvement in ANN performance compared to simple ANN model alone.

## Other Powerful ANN Models in Materials Applications

The other powerful and efficient neural network models rather than multilayer BPNN have also brought successful prediction results in recent works to determine the tensile mechanical properties of materials. Yilmaz and Ertunc (2007) [[49](#_ENREF_49)] introduced a neural network model, named generalized regression neural network (GRNN), to predict tensile strength of steel wires by using all the production parameters (the amount of carbon, ferrite and inclusions) and the diameter of steel wires. That approach was constructed with four layers: input layer, a layer of radial basis centers, a linear layer of regression unit and the output layer. A very good statistical performance with a 0.96 correlation coefficient between the target data and the predicted output have demonstrated the result of good agreement to determine the tensile strength of steel with high accuracy and reliability.

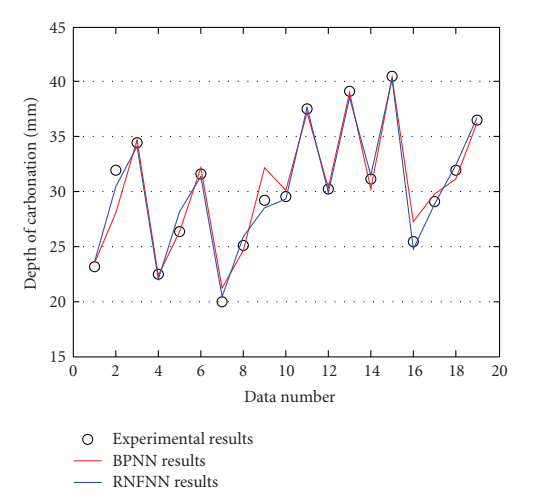
Kappatos et al., (2010) [[22](#_ENREF_22)] adopted a radial basis function (RBF) neural network, one of the mostly used feed forward network models after multilayer network, to assess the effect of existing corrosion damage on the tensile behaviour of the wrought magnesium alloy AZ31 by predicting the time dependency of the tensile mechanical properties degradation. The data used to train the network was derived from extensive experimental investigation. The authors used only two input parameters (pit depth and pitting density) that had stronger discriminant capability on output (elongation of fracture and ultimate tensile strength). Although there was no need to determine the number of hidden layers for RBF, extensive trials were carried out to determine the optimum number of hidden neurons to achieve the best prediction accuracy. Conventional linear modelling techniques fully optimized the simple linear transformation at the output layer of RBF network. Greater RBF networks with 40 and 20 hidden neurons gave higher prediction accuracy from 99.61% to 99.83% for elongation of fracture and from 99.27% to 99.68% for ultimate tensile strength, respectively. ANN results made a comparison between two input parameters to find their impact on the output such that more accurate output tensile strength was achieved with pitting density while the pit depth had stronger effect on the decrease of the mechanical properties than pitting density. RBF neural network prediction results were very good agreement with experimental results.

Most of successful materials-related ANN researches have been done with multilayer BPNN. Here, it can be found that other ANN types are as powerful and efficient as multilayer BPNN in prediction performance. Regarding to physical background of the problem, input parameters should be selected as important features that have a strong relation with output parameters so that computational cost and size of training data can be reduced to improve the prediction performance.

## ANN Models in Comparison and Hybrid ANN Models

In some literatures, ANN prediction result was compared to not only experimental results but also other feed forward ANN models’ results. In turning process, to control the desired surface roughness by manufacturing makes high expense. To establish a functional relationship between process parameters of turning process and surface roughness, MLP neural networks have been mostly implemented for a decade. But MLP needs to determine the number of hidden layers and hidden neurons in each layer with a costly trial-and-error approach. Unlike MLP, as radial basis function (RBF) neutral network has the advantage of having only one hidden layer and the number of hidden neurons can automatically be adjusted in learning algorithm, less computational time and simpler training can give faster and more accurate results. Sonar et al., (2005) [[63](#_ENREF_63)] used the advantage of RBF neural network to construct a predictive model for the surface roughness of mild steel with process parameters (feed rate (*f*), cutting speed (*v*), depth of cut (*d*) and acceleration of radial vibration (*a*)) in a turning process by HSS (high speed steel) and carbide tools, and its performance was compared with the reported performance of a MLP neural network by Kohli and Dixit [[83](#_ENREF_83)] as well as experimental results. The RBF neural network has been implemented for predicting the most likely estimate as well as the upper and lower estimate, calculated by fuzzy linear interval regression model, of surface roughness. The results showed that experimental values exist between the range of the lower and upper estimate and the most likely estimate in most cases is close to experimental values. Also, compared to MLP, the root mean squares errors of RBF are nearly the same as MLP. But RBF made slightly inferior performance against MLP with less computational time, and the errors were more than 20% with a few testing data, but still reasonable results were given. The authors discussed about increasing the number of training and testing data to increase the network accuracy.

Another similar comparison of different ANN models was found in [[62](#_ENREF_62)]. Lu and Liu (2009) analyzed the carbonation depth of prestressed concrete under different stress states by adopting two feed forward ANNs, BPNN and RBFNN with concrete mixture parameters, together with comparison in their performance and comparison with experimental results as well. Training data and test data for two ANNs were produced by an accelerated carbonation practical experiment of prestressed concrete. The 5-10-1 structure of BPNN is the optimal network structure for prediction. RBFNN was also established with the same number of input and output parameters. RBFNN results have the largest absolute percentage error of 8.46% whereas the largest absolute percentage error of BPNN is 10.88%. In this work, although RBFNN gave better precision than BPNN, the precision level of BPNN can be improved by adding the number of hidden layers appropriately that will lead to a costly trial-and-error approach. Because the error rates of both models were acceptable and their estimation results were good agreement with experimental results shown in Fig. 5, ANN has a high generalization ability to analyze and predict carbonation depth in concrete. The authors suggested that RBFNN is a better model for predicting carbonation depth in concrete and solving other civil engineering related problems as well. However, they reported that enough training and testing data was still needed to construct a perfect ANN for providing a new practical approach to concrete carbonation analysis.



**Fig 5.** Relationship between the two ANNs’ training and testing results and the experiment results in [[62](#_ENREF_62)]

From previous works, it is inevitable that different ANN analytical models based on artificial intelligence can yield somewhat reasonable, acceptable and satisfactory results. Besides, not only single ANN alone but also hybrid ANN (that combines two or more different ANNs) can give reasonable and acceptable results for prediction. That fact was supported by Li et al., (2017) [[57](#_ENREF_57)] who established a hybrid ANN (HNN) composed of one BP and one RBF by combining their advantages to construct an optimal ANN prediction model. The tribological properties of solid lubricants reinforced nano-TiO2/polyamide6 composites (friction coefficient and ware rate) were analyzed as a function of material composition, testing loads, and velocities. In this work, adaptive genetic algorithm (AGA), that computes the optimal number of hidden neurons and mixed coefficients of BP and RBF, was also coupled with HNN to improve network prediction performance by covering the disadvantages of genetic algorithm (GA) of being prone to premature and slow to converge. The HNN could estimate the tribological properties with high accuracy of under 5% small relative errors and over 0.99 high correlation index and establish the relationship of tribological properties and process parameters so that exhausted experimental work can be dramatically reduced for future prediction.

However, there is no defined universal ANN model that always outperforms on other ANN models. The right choice of ANN model should be made in accordance with the problem to be solved at hand. The network performance relies on the level of complexity and nonlinearity of input-output mapping as well as the amount of training and testing data and network topology (such as learning rate, learning algorithm, number of hidden layers, activation function and number of hidden neurons). Moreover, to make a result comparison with experimental results for optimal result, ANN models must be trained and tested with the same data set as experimental model.

## Summary

Materials data are becoming so abundant that their relationship is quite complicated to handle well. Traditional linear regression analysis is mostly not able to handle a large number of variables and nonlinear relationship among them. The main benefit of ANN over conventional regression analysis is that ANN can model problems in which there is no clear relationships between inputs and outputs and construct the solutions that can not be easily formulated within short time without specifying the form of interactions between variables. From previous works, it can be said that ANN is a good estimator for materials related problems against statistical linear regression analysis due to its advantages of fault-tolerance, noise-tolerance and generalization ability. It can solve both nonlinear and linear problems with high accuracy. As a disadvantage, although ANN has benefit of parallel structure, it sometimes spends long training and operating time and occurs instability when applied to larger problems. Important features that have a strong relation with output parameters should carefully be selected as input into ANN training such that unnecessary computational overhead and increased size of training data can be reduced to attain high classification performance.

But it is critical to be noted that misuse of over-complicated networks cannot give the optimal results. ANN should be correctly implemented according to types of problems to be solved to avoid the misuse of ANN benefit. If the number of hidden neurons, compared to the number of data pairs in evaluating the fitting parameters, are not enough as in [[67](#_ENREF_67)] [[84](#_ENREF_84)] or more redundant as in [[43](#_ENREF_43)], it will lead to the misuse of ANN. Moreover, it does not mean the more complicated the networks, the better the results. The number of neurons in hidden layers of neural networks should also be increased within a limit depending on the problem, otherwise; mathematically undefined situation, known as overfitting, in which determining more fitting parameters than the available data points is difficult, will make poor network generalization ability on unseen data. The joint implementation of ANN and other computing paradigms should further be considered due to their good cooperation results.

# Trends of the ANN application in materials area

At present, researchers are trying to implement ANN models to predict the performance, stability and structure of materials that is also a great challenge in materials science. According to [[85](#_ENREF_85)], in 2020, materials industries, that supply steel, petrochemical products, cement, etc., will be the key technology of automotive industry to develop new structural materials. ANN can accelerate the design of new materials by predicting material properties with high accuracy. To combine materials science with computer science by ANN prediction for materials properties is a great solution for researchers not only at present but also in future.

Previous works described their network parameters: network structures, training algorithms, transfer functions and data used to train and test ANN, in related researches so that those works can be expanded and enhanced by new researchers. Since their prediction results gave satisfactory and acceptable outcomes against experimental results, ANN prediction models can significantly reduce the quantitative experimental works. But most recent works showed large amount of data are still needed to train ANN. ANN performance can be extended when there is data big enough for constructing an optimized neural network model and then the prediction results will be more exact for future use. Since ANN has the abilities of noise-tolerence and fault-tolerence, it can deal well with real-world data that are somewhat noisy, uncertain, complex and missing, and is the whole solution to complicated problems to give the satisfactory result.

Most neural network models in context of materials science are feed forward types and other popular, powerful and efficient feedback neural networks (Recurrent Neural Network, Long/Short Term Memory Neural Network, etc.), that are currently widely implemented in image and video recognition, time series prediction, handwriting recognition, speech recognition, automated robotics and machine translation applications in computer science researches, and hybrid use of different network types would be future research trends in materials science too. It is still necessary to conduct more researches related with those networks in materials related fields to give strongly recommended results to new researchers. And also, by using input ranking methods that made a great contribution to ANN performance, unnecessary input parameters will easily be removed from ANN model to become more simpler model that can give more fruitful results. Hence, the implementation of ANN in the prediction of material properties may achieve higher score and find more application prospects in the future.

The purpose of this paper is to reveal the significance of ANN in many aspects of materials related problems and it can be seen that ANN prediction accuracy was apparently improved in recent researches compared to traditional statistical regression equations. It is expected that this paper can give a hand to materials researchers with a comprehensive review of some applications of neural network in the context of materials science.

# Acknowledgements

We also thank the financial support from the Ministry of Science and Technology, China for the national key research and development plan (2017YFB0701904). And the authors are also grateful for support from the 111 Project (Grant No. B12012) in China for promoting international exchange.

# Appendix

**Nomenclature**

The following were alphabetically ordered.

*a*  acceleration of radial vibration

Ag Silver

Al aluminum

B binder

B3(OH)3 boron content

Bi Bismuth

BSW Basic Saturated Water

C carbon

C/CA cement-coarse aggregate ratio

Cd current density

C/FA cement-fine aggregate ratio

CEIIW carbon equivalent

CEPcm carbon equivalent based on the Ito-Bessyo equation

CGR crack growth rate

Cl- chloride ions concentration

Cr chromium

CrMoNiCu the sum of chromium, molybdenum, nickel and copper concentrations

Csic SiC particle concentration

Cu copper

*d* (or) t depth of cut

DC depth of carbonation

Dmax maximum pit depth

E potential

Ecorr corrosion potential

ECP principal environmental factor

El elongation

*f* (or) s feed rate

FCGR fatigue crack growth rate

Fe Iron

H2SO4  sulfuric acid

HCl hydrochloric acid

HP high pressure

icorr corrosion current density

In Indium

KI  principal mechanical factor

Li lithium content

MK metakaolin addition

Mn magnesium

Mo molybdenum

N nitrogen

NaCl chloride ion

Nb niobium

NbV the sum of niobium and vanadium concentrations

Ni nickel

P applied stress

P Phosphorus

PCO2 pressure of purged CO2

PO2 relative pressure of oxygen

PTFE Polytetrafluoroethylene

Q charge amount

planar anisotropy

Ra surface roughness

Re Rhenium

RH relative humidity

Rp polarization resistance

S strain

S Sulfur

Sb antimony

SCC stress corrosion cracking

Si Silicon

SIF stress intensity factor

SL stress level of concrete

Sn Tin

SO2 sulphur dioxide

SP superplasticizer

SR strain rate

T temperature

TA testing age

Ti titanium

TiO2 titanium dioxide

TOW time of wetness

Up ultrasonic power

UTS ultimate tensile strength

UV ultrasonic velocity

V vanadium

*v* cutting speed

VTiNb the sum of niobium, vanadium and titanium concentrations

W sample weight change

w frequency

W/B water-to-binder ratio

W/C water-cement ratio

WV wind velocity

YS yield strength

Zr and Zi real and imaginary impedances

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