

Neural Networks in Materials Science and Engineering: A Review of Salient Issues

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ABSTRACT

The paper 'Neural Networks in Materials Science and Engineering: A Review of Salient Issues' has been extensively reviewed. The paper has explained neural networks and had clearly presented it as a powerful predictive tool that can be trained to solve very complex problems in materials Science and Engineering. Attempts have also been made at comparing linear regression model with neural networks and the findings are that neural networks are more sophisticated in terms of providing solutions to materials science and engineering problems than linear regression model. The paper has revealed that neural networks have found wide applications in materials science and engineering particularly in solving very complex problems: problems with established theories but the quantitative determination was lacking because of so many independent and interacting parameters. Finally the paper concluded by raising some salient issues that had to do with the use of neural networks in materials science and engineering. One of such issues is them is application of neural network methodologies, thereby limiting their potential benefit.

Keywords:Materials science, Engineering, Application, Neural networks, Salient issues, Artificial.

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INTRODUCTION

There are difficult problems in materials science where the general concepts might be understood but which are not as yet amenable to scientific treatment. We are at the same time told that good engineering has the responsibility to reach objectives in a cost and time-effective way. Any model which deals with only a small part of the required technology is therefore unlikely to be treated with respect. Neural network analysis is a form of regression or classification modeling which can help resolve these difficulties whilst striving for longer term solutions [1].

Rouse [2] said "in information technology, a neural network is a system of programs and data structures that approximates the operation of the human brain. A neural network usually involves a large number of processors operating in parallel each with its own small sphere of knowledge and access to data in its local memory. According to Fausett [3] an artificial neural network is an information-processing system that has certain performance characteristics in common with biological neural networks. Graupe [4] said Artificial neural networks are, as their name indicates, computational networks which attempt to simulate, in a gross manner, the networks of nerve cell (neurons) of the biological (human or animal) central nervous system. This simulation is a gross cell-by-cell (neuron-by-neuron, element-by-element) simulation. Yu [5] artificial neural network (ANN) is a kind of imitation of the biological brain structure and the function of information management system which was developed in the 1980s. The researcher gave a high rating of the model particularly its ability to solve even nonlinear problems.

Neural Network (NN) has emerged over the years and has made remarkable contribution to the advancement of various fields of endeavor. Whenever we talk about a neural network, we should more properly say "artificial neural net-work" (ANN), because that is what we mean most of the time [6]. Artificial neural networks are computers whose architecture is modeled after the brain. They typically consist of many hundreds of simple processing units which are wired together in a complex communication network. Each unit or node is a simplified model of a real neuron which fires (sends off a new signal) if it receives a sufficiently strong input signal from the other nodes to which it is connected. Artificial neural networks are, as their name indicates, computational networks which attempt to

simulate, in a gross manner, the networks of nerve cell (neurons) of the biological (human or animal) central nervous system [6]. This simulation is a gross cell-by-cell (neuron-by-neuron, element-by-element) simulation. It borrows from the neuro-physiological knowledge of biological neurons and of networks of such biological neurons. It thus differs from conventional (digital or analog) computing machines that serve to replace, enhance or speed-up human brain computation without regard to organization of the computing elements and of their networking. Humans are born with as many as 100 billion neurons, see fig. 1 for the illustration of a biological neuron. Most of these are in the brain, and most are not replaced when they die, in spite of our continuous loss of neurons, we continue to learn. Even in cases of traumatic neural loss, other neurons can sometimes be trained to take over the functions of the damaged cells. In similar manner, artificial neural network can be designed to be insensitive to small damage to the network, and the network can be retrained in cases of significant damage (e.g. loss of data and some connections).

An Artificial Neural Network (ANN) is an information processing paradigm that is inspired by the way biological nervous systems, such as the brain, process information. The key element of this paradigm is the novel structure of the information processing system. It is composed of a large number of highly interconnected processing elements (neurons) working in unison to solve specific problems. ANNs, like people, learn by example. According to Michael Mozer of the University of Colorado, "The neural network is structured to perform nonlinear Bayesian classification" A neural network could also be described as a system composed of many simple processing elements operating in parallel whose function is determined by network structure, connection strengths, and the processing performed at computing elements or nodes [7].

It resembles the brain in two respects: 1. Knowledge is acquired by the network through a learning process.

2. Interneuron connection strengths known as synaptic weights are used to store the knowledge [6].

Neural networks are now a prominent feature of materials science with rapid progress in all sectors of the subject. It is premature, however, to claim that the method is established. There are genuine difficulties caused by the often incomplete exploration and publication of models. The development and processing of materials is complex. Although scientific investigations on material have helped greatly in understanding the underlying phenomena, there remain many problems where quantitative treatments are dismally lacking. For example, whereas dislocation theory can be used to estimate the yield strength of microstructure, it is not yet possible to predict the strain hardening coefficient of an engineering alloy. It follows that the tensile strength, elongation, fatigue life, creep life and toughness, all of which are vital engineering design parameters, cannot even be estimated using dislocation theory. A more comprehensive list of what needs to be done in this context is presented in Table 1[8].

Table 1. Mechanical properties that need to be expressed in quantitative models as a function of large numbers of variables.

Property	Relevance
Yield strength	All structural applications
Ultimate tensile strength	All structural applications
YS/UTS ratio	Tolerance to plastic overload
Elongation	Resistance to brittle fracture
Uniform elongation	Related to YS and UTS
Non-uniform elongation	Related to inclusions
Toughness	Tolerance to defects
Fatigue	Cyclic loading, Life assessments
Stress corrosion	Slow corrosion & cracking
Creep strength	High temperature service
Creep ductility	Safe design
Creep-fatigue	Fatigue at creep temperatures
Elastic modulus	Deflection, stored energy
Thermal expansivity	Thermal fatigue/stress/shock
Hardness	Tribological properties
Age hardening heat treatment	Ageing time and temperature
Sand mould preparation	Mould strength and other properties

The lack of progress in predicting mechanical properties is because of their dependence on large numbers of variables, Nevertheless, there are clear patterns which experienced metallurgists recognize and understand. For example, it is well understood that the toughness of steel can be improved by making its microstructure more chaotic so that propagating cracks are frequently deflected. It is not clear exactly how much the toughness is expected to improve, but the qualitative relationship is well established on the basis of a vast number of experiments. Neural network models are extremely useful in such circumstances, not only in the study of mechanical properties but wherever the complexity of the problem is overwhelming from a fundamental perspective and where simplification is unacceptable. There are many established theories in materials science and engineering that have been proven empirically through several experiments but are difficult to predict using simple linear and multiple linear regression models: artificial neural networks comes handy in such situations [9].

The objective of this review is to outline some areas of application of artificial neural network in materials science and engineering and to raise salient issues associated with the application.

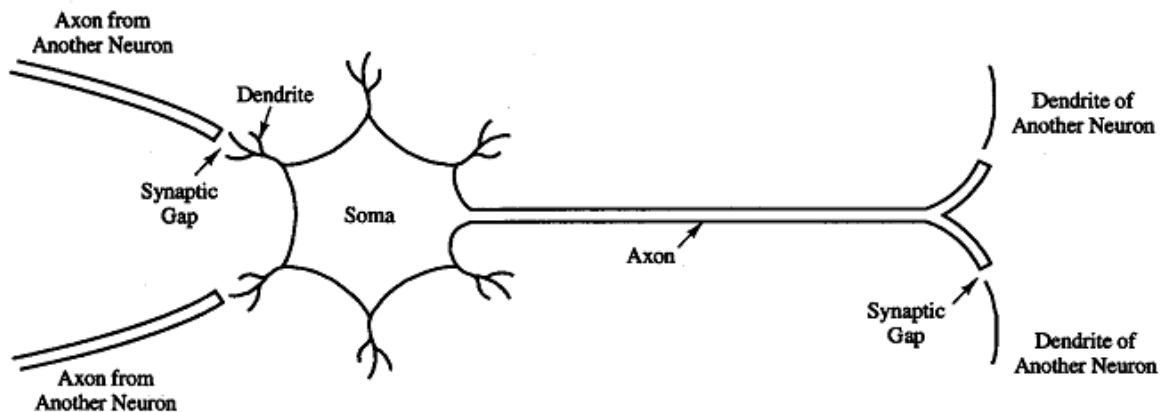


Fig. 1 Biological neuron [4]

PHYSICAL AND EMPIRICAL MODELS

There have been some established theories in materials science and engineering like the relationship between porosity and thermal conductivity or the relationship between clay content and the strength of a moulding sand mixture. The theories of these relationships have been well studied and proven empirically through instrumental measurements. However, as Bhadeshia [1] puts it; A good theory must satisfy at least two criteria. It must describe a large class of observations with few arbitrary parameters. And secondly, it must make predictions which can be verified or disproved. Physical models, such as the crystallographic theory of marten site, satisfy both of these requirements. Thus, it is possible to predict the habit plane, orientation relationship and shape deformation of marten site with a precision greater than that of most experimental techniques, from knowledge of just the crystal structures of the parent and product phases. By contrast, a linear regression equation requires at least as many parameters as the number of variables to describe the experimental data, and the equation itself may not be physically justified. Neural networks fall in this second category of empirical models; we shall see that they have considerable advantages over linear regression. In spite of the large number of parameters usually necessary to define a trained network, they are useful in circumstances where physical models do not exist [1].

Linear Regression

Linear regression is normally used to determine the best line of fit for a graphical model where you have the dependent variable (y) and independent variable(x). It provides the best fit for the empirical values and therefore can be used for prediction purposes [9, 10]. Simple linear regression is used when the independent variable is one, but when the number of independent variables is in multiple of one and above, multiple linear regressions is used. As the name implies linear regression applies to phenomena that are linear, predictions become inaccurate when the behavior of the system changes and becomes nonlinear. For instance in the elastic deformation of a material once the elastic limit is exceeded the relationship between the stress and strain changes, in like manner in the strength –carbon relationship in steel as the carbon content in steel is increased the strength is increased but there comes a point when the steel will change to cast iron and the properties also change. In instances like these linear regression

becomes inadequate as a prediction model. Equation 1 shows a typical simple linear regression equation expressing the relationship between hardness (y) the dependent variable, and distance below the surface of quenched carbon steel (x) the independent variable [9].

$$Y(H) = 946.57 - 156.56X(1)$$

Equation 2 is an example of a multiple linear regression model. The developed mathematical model for the relationship between bulk density and the two variables of clay and moisture content where Bulk density is Y_2 ; Clay content is X_1 ; and Moisture content is X_2 [10].

$$Y_2 = 1.48 + 0.09X_1 - 0.059X_2 \quad (2)$$

Though multiple regression equation may make provision for interacting variables, when the number of variables becomes so many computation also becomes difficult and by implication the accuracy of the result. This is because some dependent variables may depend on several independent variables. According to Bhadeshia [1] of course, there is no justification for the choice of the particular form of relationship. This and other difficulties associated with ordinary linear regression analysis can be summarized as follows:

Difficulty (a) A relationship has to be chosen before analysis.

Difficulty (b) the relationship chosen tends to be linear, or with non-linear terms added together to form a pseudo-linear equation.

Difficulty (c) The regression equation, once derived, applies across the entire span of the input space. This may not be reasonable. For example, the relationship between strength and the carbon concentration of an iron-base alloy must change radically as steel gives way to cast iron.

The main advantages of ANN as compared to multiple regression model include: 1) ANN does not require any prior specification of suitable fitting function, and 2) ANN also has a universal approximation capability to approximate almost all kinds of non-linear functions including quadratic functions, whereas multiple regression model is useful only for quadratic approximations. There are some studies in the literature where model were developed based on multiple regression model and ANN using the same experimental design. For example, Elmabrouk and Kalkanli, [11] reported the comparison of ANN and multiple regression model in the lipase-catalyzed synthesis of palm-based wax ester, and they suggested the superiority of ANN over multiple regression model. Both the ANN and multiple regression model techniques were recently compared for their predictive and generalization capabilities, sensitivity analysis and optimization efficiency in fermentation media optimization. It was found that the ANN predicted model has higher accuracy and better generalization capability than multiple regression model, even with the limited number of experiments. In another study, the multiple regression model and ANN methodologies were applied for predicting the amount of zinc by flame atomic absorption spectrometry (FAAS) in fish samples. The results which were obtained through multiple regression model were then compared with those through ANN and the same conclusion as the preceding above was drawn [11].

NEURAL NETWORKS

Historical Background

The development of artificial neural networks began approximately 50 years ago, motivated by a desire to try both to understand the brain and to emulate some of its strengths. Early successes were overshadowed by rapid progress in digital computing. Also, claims made for capabilities of early models of neural networks proved to be exaggerated, casting doubts on the entire field. Recent renewed interest in neural networks can be attributed to several factors. Training techniques have been developed for the more sophisticated network architectures that are able to overcome the shortcomings of the early, simple neural nets. High-speed digital computers make the simulation of neural processes more feasible. Technology is now available to produce specialized hardware for neural networks. However, at the same time that progress in traditional computing has made the study of neural networks easier, limitations encountered in the inherently sequential nature of traditional computing have motivated some new directions for neural networks research. Fresh approaches to parallel computing may benefit from the study of biological neural systems which are highly parallel [4]. The history of neural networks can be divided into several periods: from when developed models of neural networks based on their understanding of neurology, to when neuroscience became influential in the development of neural

networks. Psychologists and engineers also contributed to the progress of neural network simulations. Neurally based chips are emerging and applications to complex problems are being developed. Clearly, today is a period of transition for neural network technology [6]

Architecture of Neural Networks

The arrangement of neurons into layers and the connection patterns within and between layers is called the net architecture. Many neural nets have an input layer in which the activation of each unit is equal to an external input signal. The net illustrated in fig. 2 consists of input units, output units, and one hidden unit (a unit that is neither an input unit nor an output unit).

Neural nets are often classified as single layer or multilayer. In determining the number of layers, the input units are not counted as a layer, because they perform no computation. Equivalently, the number of layers in the net can be defined to be the number of layers of weighted interconnected links between the slabs of neurons. This view is motivated by the fact that the weights in a net contain extremely important information. The net shown in fig.3 has two layers of weights. The single-layer and multi-layer nets illustrated in fig.4 and fig. 5 are examples of feed-forward nets- nets in which the signals flow from the input units to the output units, in a forward direction. The fully interconnected competitive net in fig.6 is an example of a recurrent net, in which there are closed-loop signal path from a unit back to itself.

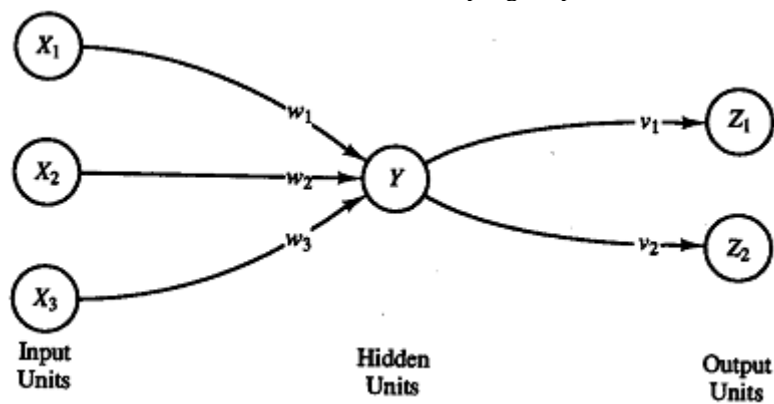


Fig.2 A Very Simple Neural Network [4]

Concept of Neural Network

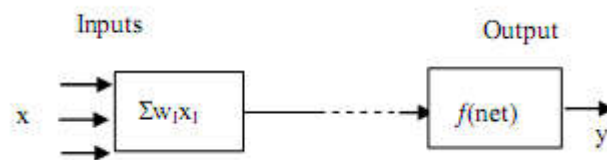


Fig.3 Concept of Neural Network [11]

The neural network resembles biological nervous systems, is a parallel distributed information-processing system that consists of processing elements called nodes interconnected by the signal channels called connections. The output of each node can be connected to the input of other nodes via these connections. Each connection has an associated weight that determines the strength of the signal passed along the connection [11]. Such networks are programmed by applying training patterns that fix the output states of the nodes. A learning algorithm then adjusts the connection weights in response to the training patterns where

$$\text{net} = w_1x_1 + w_2x_2 + w_3x_3 \tag{3}$$

The weighted sum of the inputs are sent through various layers of nodes to the output node. The activation function of the net $f(\text{net})$ is then compared with the pre-determined threshold value θ . The output node will give an output signal if activation function is greater than the threshold value.

$$f(\text{net}) = y \tag{4}$$

$$Y = \begin{cases} 1 & \text{if } a > \text{or } = \theta \\ 0 & \text{if } a < \theta \end{cases} \quad (5)$$

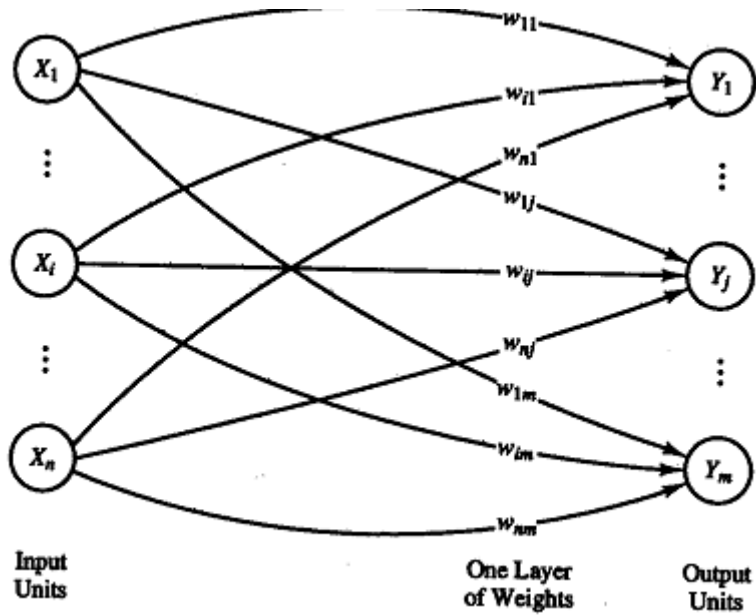


Fig.4 A Single- Layer Neural Net [4]

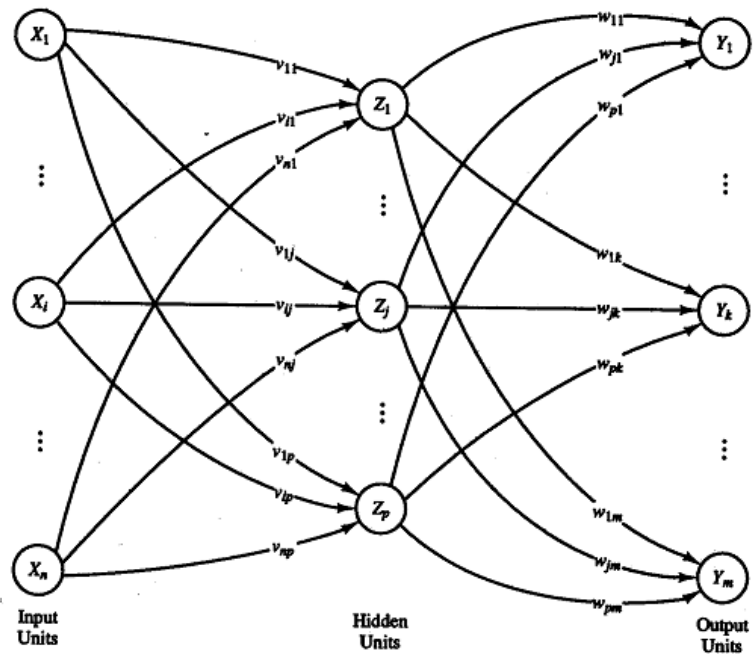


Fig. 5 A Multilayer Neural Net [4]

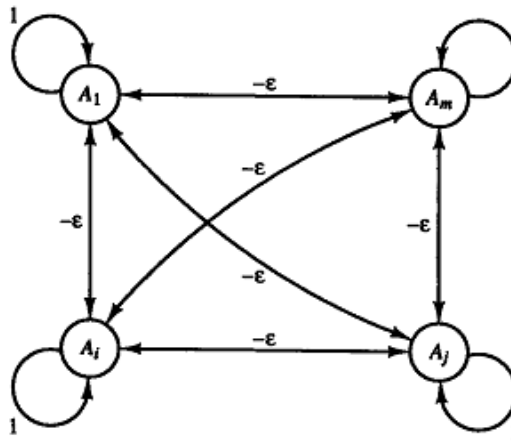


Fig. 6. Competitive Layer [4]

Single-Layer Net

A single -layer net has one layer of connection weights. Often, the units can be distinguished as inputs units, which receive signals from the outside world, and output units, from which the response of the net can be read. By contrast, the Hopfield net architecture, shown in fig.7 is an example of a single-layer net in which all units function as both input and output units.

Multilayer Net

A multilayer net is a net with one or more layers (or levels) of nodes (the so called hidden units) between the inputs units and the output units. Typically, there is a layer of weights between two adjacent levels of units (input, hidden, or output). Multilayer nets can solve more complicated problems than can single-layer nets, but training may be more difficult. However, in some cases, training may be more successful, because it is possible to solve a problem that a single layer net cannot be trained to perform correctly at all.

Competitive Layer

A competitive layer forms a part of a layer number of neural networks. Typically, the interconnections between neurons in the competitive layer are not shown in the architecture diagrams for such nets. An example for the architecture for a competitive layer is given in fig.6, the competitive interconnections have weights of $-\epsilon$.

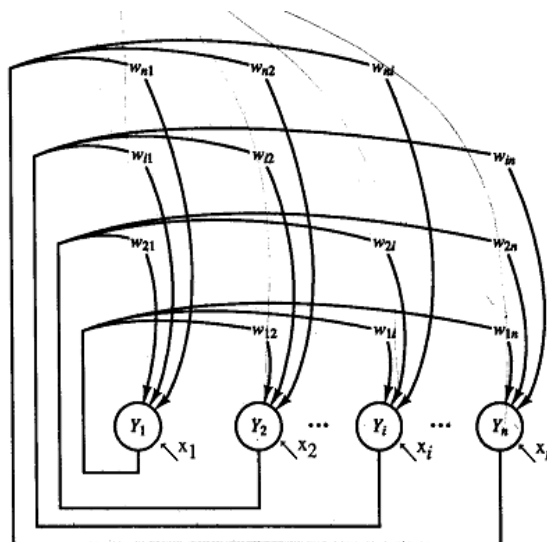


Fig.7 Discrete Hopfield Net [4]

Setting the Weights

In addition to the architecture, the method of setting the values of the weights (training) is an important distinguishing characteristic of different neural nets. For convenience, we shall distinguished two types of

training- supervised and unsupervised- for a neural network; in addition, there are nets whose weights are fixed without an iterative training process.

Supervised Training

In perhaps the most typical neural net setting, is accomplished by presenting a sequence of training vectors, or patterns, each with an associated target output vector. The weights are then adjusted according to a learning algorithm. This process is known as supervised training.

Unsupervised Training

Self-organizing neural nets group similar input vectors together without the use of training data to specify what a typical member of each group looks like or to which group each vector belongs. A sequence of input vectors is provided, but no target vectors are specified. The net modifies the weights so that the most similar input vectors are specified. The net modifies the weights so that the most similar input vectors are assigned to the same output (cluster) unit. The neural net will produce an exemplar (representative) vector for each cluster formed [4].

The back-propagation algorithm

In order to train a neural network to perform some task, we must adjust the weights of each unit in such a way that the error between the desired output and the actual output is reduced. This Process requires that the neural network compute the error derivative of the weights (EW). In other words, it must calculate how the error changes as each weight is increased or decreased slightly. The back propagation algorithm is the most widely used method for determining the EW

NEURAL NETWORKS APPLICATIONS IN MATERIAL SCIENCE AND ENGINEERING

Neural networks have had a significant impact on the development of materials and associated processes. This is because they represent a transparent and quantitative method which is able to deal with sophisticated problems typical in materials science [1]. Below are some of the areas of applications of neural networks in material science and engineering. The list of problems in materials science and engineering that can be solved using neural networks is in-exhaustible.

Effect of Quartz and Heat Treatment on the Corrosion Properties of Ceramic Coating

Elmabrouk and Kankali, [11] studied the effect of quartz and heat treatment on the corrosion properties of ceramic coating using neural network the result of which they compared with results they earlier on got using multiple linear regression. According to the researchers prediction of the effects of various heat treatments at temperatures (500,550, and 600°C) at different times (60 &120)min and with quartz addition in the range (0-15)% on the acid corrosion rate of the resultant coating of low carbon alloyed steel with (0.2)%C was achieved by using artificial neural network (ANN).

In the work two models were developed for predicting the acid corrosion rate and these were Multiple linear regression model and artificial neural network (ANN). First, multiple regression model was used for predicting the amount of acid corrosion rate. Then, the independent variables, namely heat treatments temperatures, addition times, and with quartz addition were fed as inputs to an artificial neural network, while the output of the network was the acid corrosion rate. A multilayer feed-forward network was trained by the sets of input-output patterns using quick propagation algorithm. Finally, the two methodologies were compared for their predictive capabilities. Their work indicated that the ANN was much more accurate in predicting the acid corrosion rate in comparison to the multiple linear regression model .

Thin Films and Superconductors

A lot of the materials science type issues about thin films naturally involve deposition and characterization. The deposition process can be very complicated to control and is ideally suited for neural network applications. Neural networks have been used to interpret Raman spectroscopy data to deduce the superconducting transition temperature of YBCO thin films during the deposition process; to characterize reflection high-energy electron diffraction patterns from semiconductor thin films in order to monitor the deposition process, to rapidly estimate the optical constants of thin films using the computational results of a physical model of thin films, and there are numerous other similar examples.

There is one particular application which falls in the category of "alloy design"; Asada,*et al*,[12]. Bhadeshia, [8] trained a neural network on a database of $(Y_{1-x}Ca_x)Ba_2Cu_3O_z$ and $Y(Ba_{2-x}Ca_x)Cu_3O_z$, where z 'is generally less than 7, the ideal number of oxygen atoms. The output parameter was the superconducting transition temperature as a function of x and z . They were thus able to predict the transition temperature of $YBa_2Cu_3O_z$ doped with calcium. It was demonstrated that the highest temperature is expected for $x=0.3$ and $z=6.5$ in $(Y_{1-x}Ca_x)Ba_2Cu_3O_z$ whereas a different behaviour occurs for $Y(Ba_{2-x}Ca_x)Cu_3O_z$.

Composites

There are many applications where vibration information can be used to assess the damage in composite structures e.g. Acoustic emission signals have been used to train a neural network to determine the burst pressure of fiberglass epoxy pressure vessels. There has even been an application in the detection of cracks in eggs. One different application is in the optimization of the curing process for polymer-matrix composites made using thermosetting resins.

An interesting application is the modeling of damage evolution during forging of AlSiC particle reinforced brake discs. The authors were able to predict damage in a brake component previously unseen by the neural network model. Hwang et al in Bhadeshia [1] compared prediction of the failure strength of carbon fibre reinforced polymer composite, made using a neural network model, against the Tsai-Wu-theory and an alternative hybrid model. Of the three models, the neural network gave the smallest root-mean square error. Nevertheless, the earlier comments about the validity of the neural network in extrapolation etc. remain as a cautionary note in comparisons of neural and physical models.

Steel Processing and Mechanical Properties

Hot Rolling

The properties of steel are greatly enhanced by the rolling process. It is possible to cast steel into virtually the final shape but such a product will not have the quality or excellence of a carefully rolled product. Singh *et al*, in Bhadeshia [1] have developed a neural network model in which the yield and tensile strength of the steel is estimated as a function of some 108 variables, including the chemical composition and an array of rolling parameters. Implicit in the rolling parameters is the thermal history and mechanical reduction of the slab as it progresses to the final product. The training data come from sensors on the rolling mill. There is therefore no shortage of data, the limitation in this case being the need to economize on computations. There are some exciting results which make sense from a metallurgical point of view, together with some novel predictions on a way to control the yield to tensile strength ratio.

A similar model by Korczak *et al*, [13] uses microstructural parameters as inputs and has been applied to the calculation of the ferrite grain size and property distribution through the thickness of the final plate.

Vermeulen *et al*, [15] have similarly modeled the temperature of the steel at the last finishing stand. They demonstrated that it is definitely necessary to use a non-linear representation of the input variables to obtain an accurate prediction of the temperature. The control of strip temperature on a hot strip mill run out table has also been modeled by Loney, *et al*, [14].

Heat Treatment

A Jominy test is used to measure the hardenability of steel during heat treatment. Vermeulen *et al*, [15] have been able to accurately represent the Jominy hardness profiles of steels as a function of the chemical composition and austenitising temperature.

Mechanical Properties

There are many other examples of the use of neural networks to describe the mechanical properties of steels; Dumortier *et al*, in Bhadeshia [8] have modeled the properties of micro-alloyed steels; Milykoski, in Bhadeshia [8] has addressed the problem of strength variations in thin steel sheets; microstructure property relationships of C-Mn steels, the tensile properties of mechanically alloyed iron with a comparison with predictions using physical models; and the hot-torsion properties of austenite.

Polymeric and Inorganic Compounds

Neural network methods have been used to model the glass transition temperatures of amorphous and semi-crystalline polymers to an accuracy of about 10K, and similar models have been developed for relaxation temperatures, degradation temperature, refractive index, tensile strength, elongation, notch strength, hardness, etc. The molecular structure of the monomeric repeating unit is described using topological indices from graph theory. The techniques have been exploited, for example, in the design of polycarbonates for increased impact resistance. In another analysis, the glass transition temperature of linear homopolymers has been expressed as a function of the monomer structure, and the model has been shown to generalize to unseen data to an accuracy of about 35K [3].

Comparison with Quantum Mechanical Calculations

There is an interesting study which claims that neural networks are able to predict the equilibrium bond length, bond dissociation energy and equilibrium stretching frequency more accurately, and far more rapidly than quantum mechanical calculations. The work dealt with diatomic molecules such as LiBr, using thirteen inputs: atomic number, atomic weight (to include isotope effects), valence electron configuration (s,p,d, f electrons) for both atoms, and the overall charge. The corresponding quantum

mechanical calculations used effective core potentials as inputs. It was found that all three molecular properties could be predicted more accurately using neural networks, with a considerable reduction in the computational effort. Such a comparison of a physical model with one which is empirical is not always likely to be fair. In general, an appropriate neural network model should perform Badly when compared with a physical model, when both are presented with precisely identical data. This is because the neural network can only learn from the data it is exposed to. By contrast, the physical model will contain relationships which have some justification in science, and which impose constraints on the behaviour of the model during extrapolation. As a consequence, the neural network is likely to violate physical principles when used without restriction. The continuous cooling transformation curve model is an example where the neural network produces information in forbidden domain and produces jagged curves, which a physical model using the same data would not because the form of the curves would be based on phase transformation theory [8].

Ceramics

Ceramic Matrix Composites

Ceramic matrix composites rely on a weak interface between the matrix and fibre. This introduces slip and debonding during deformation, thus avoiding the catastrophic propagation of failure. The mathematical treatment of the deformation has a large number of variables with many fitting parameters. For an Al_2O_3 matrix Sic whisker composite a constitutive law has been derived using an artificial neural network, using inputs generated by finite element analysis. Hybrid models can be created by training neural networks on data generated by physical models [3].

Machining and Processing

There are many examples where neural networks have been used to estimate machine-tool wear. For example, Ezugwu *et al.*, (1995) have modeled the tool life of a mixed-oxide ceramic cutting tool as a function of the feed rate, cutting speed and depth of cut. Tribology issues in machining, including the use of neural networks, have been reviewed by Jahanmir. Neural networks are also used routinely in the control of cast ceramic products made using the slip casting technique, using variables such as the ambient conditions, raw material information and production line settings. In another application, scanning electron microscope images of ceramic powders were digitized and processed to obtain the particle boundary profile; this information was then classified using a neural approach, with exceptionally good results even on unseen data.

REVIEW OF SALIENT ISSUES IN THE USE OF NEURAL NETWORKS IN MATERIALS SCIENCE AND ENGINEERING

Neural networks are now a prominent feature of materials science with rapid progress in all sectors of the subject. It is premature, however, to claim that the method is established. The use of computer modeling techniques is extensive in scientific research. Artificial neural networks are now well established, and prominent in the literature, when computational based approaches are involved. The materials science and engineering research community has and continues to take advantage from new developments in these areas with different applications regularly emerging, along with the degree of sophistication utilised. However, with this increased use there is unfortunately a growing tendency for the misapplication of neural network methodologies, limiting their potential benefit. Central to the problem is the use of over complicated networks that are frequently mathematically indeterminate, and by using limited data for training and testing. This problem is not unique to one particular field, but has prompted the authors to bring it to the attention of the materials and engineering research community in order to elaborate. Neural networks have proved to be powerful and popular in dealing with complex problems of the type typical in materials science and engineering. Indeed, as pointed out by Abrahart *et al.*, [17] aside from materials science, there are reviews or extended summaries of the applications of networks in the fields of hydrological sciences, atmospheric sciences, civil engineering, process engineering and structural engineering including computer and electrical/electronic engineering. This reflects the generic nature of the method. However, the way in which the method is applied varies widely and it would be useful to assess the advantages and disadvantages of the different approaches and the way in which the results are presented and published. It has previously been pointed out, when discussing neural networks in the hydro-sciences, that in many cases the model building process is described poorly, making it difficult to assess the optimality of the results obtained. The issues raised here may hopefully prevent others and potentially new researchers from continued misuse of neural networks in the future [1]. We note that at the present state of neural networks their range of adaptability

is limited. However, their design is guided to achieve this simplicity and self-organization by its gross simulation of the biological network that is (must be) guided by the same principles [4].

Recent renewed interest in neural networks can be attributed to several factors. Training techniques have been developed for the more sophisticated network architectures that are able to overcome the shortcomings of the early, simple neural nets. High-speed digital computers make the simulation of neural processes more feasible. Technology is now available to produce specialized hardware for neural networks. However, at the same time that progress in traditional computing has made the study of neural networks easier, limitations encountered in the inherently sequential nature of traditional computing have motivated some new directions for neural networks research. Fresh approaches to parallel computing may benefit from the study of biological neural systems which are highly parallel [3]. The application of neural networks in materials science is a rapidly growing field. There are numerous papers being published but the vast majority is of little use other than to the authors. This is because the publications almost never include detailed algorithms, weights and databases of the kind necessary to reproduce the work. Work which cannot be reproduced or checked goes against the principles of scientific publication. The minimum information required to reproduce a trained network is the structure of the network, the nature of the transfer functions, the weights corresponding to the optimized network and the range of each input and output variable. Such detailed numerical information is unlikely to be accepted for publication in journals. There is now a world wide website where this information can be logged for common access [8]. The major issues of concern today are the scalability problem, testing, verification, and integration of neural network systems into the modern environment. Neural network programs sometimes become unstable when applied to larger problems. The defense, nuclear and space industries are concerned about the issue of testing and verification. The mathematical theories used to guarantee the performance of an applied neural network are still under development. The solution for the time being may be to train and test these intelligent systems much as we do for humans. Also there are some more practical problems like: the operational problem encountered when attempting to simulate the parallelism of neural networks instability to explain any results that they obtain. Networks function as "black boxes" whose rules of operation are completely unknown [6].

CONCLUSION

The paper 'neural networks in materials science and engineering: a review of salient issues' has been extensively reviewed. The paper has explained neural networks and had clearly presented it as a powerful predictive tool that can be trained to solve very complex problems. Attempts have also been made at comparing linear regression model with neural networks and the findings are that neural networks are more sophisticated in terms of providing solutions to materials science and engineering than linear regression model. The paper has revealed that neural networks have found wide applications in materials science and engineering particularly in solving very complex problems: problems with established theories but the quantitative determination was lacking because of so many independent and interacting parameters. Finally the paper concluded by raising some salient issues that had to do with the use of neural networks in materials science and engineering as follows:

The application of neural networks in materials science is a rapidly growing field. The mathematical theories used to guarantee the performance of an applied neural network are still under development. The solution for the time being may be to train and test these intelligent systems much as we do for humans.

Also there are some more practical problems like: the operational problem encountered when attempting to simulate the parallelism of neural networks instability to explain any results that they obtain. Networks function as "black boxes" whose rules of operation are completely unknown. The use of the ANN is therefore subject to abuse.

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