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Virtual Metallurgy: Alloy Formation And Prediction of Their Properties Through Artificial Neural Network

Pradeep Kumar Singh [*]

Asst. Professor, Department of Mechanical Engineering
GLA University, Mathura-281406 (U.P.), India

*Corresponding Author: pradeep.kumar@gla.ac.in

ABSTRACT
In the present paper a novel concept of metallurgy viz., 'virtual–metallurgy' is introduced. With virtual metallurgy, it is possible to make a large variety of potential alloys and its properties prediction could be done through Artificial Neural Network (ANN). Using the virtual-metallurgy concept, a few new alloys are found with interesting and improved properties viz. [i] Braonze (combination of Brass & Bronze) and [ii] Hc-Hss tool material (combination of high carbon steel & high speed steel). Properties of Brass & Bronze and that of High carbon steel & High speed steel are used as training data to train the ANN.

Virtual-metallurgy in broader sense, is virtual-chemistry, and it can find wide-ranging applications towards virtual-testing & development of ***composite materials****,* ***polymers****, medicines etc. Virtual-metallurgy can be considered as eco-friendly metallurgical manufacturing process & testing, that avoids unnecessary hit and trial experiments for the alloy making, only the better ones predicted by ANN can actually be made.*

Keywords: *Virtual metallurgy, Artificial Neural Network, Alloys, Virtual Chemistry.*

I. INTRODUCTION

The important interrelated keys to industrial revolution are power, metallurgy and manufacturing. In the present paper a novel concept of metallurgy viz., 'virtual metallurgy' is proposed which can make a revolution in metallurgy and would become an indispensable tool for metallurgists.

There are many elements in periodic-table out of which many alloys could be thought of, but its combination / permutations that too with different proportions are almost infinite. All the possible potential alloys cannot be physically made or tested experimentally. But with virtual metallurgy with the help of computer, it is possible to make a very large variety of potential alloys and its properties prediction could be done through Artificial Neural Network (ANN).

Artificial Neural Network (ANN) is diagnostic, predictive and forecasting technique [1-3]. In fact, ANN is a mathematical brain with artificial intelligence which does massive interacting processing with the use of computer-software to predict output from input as natural neural network (brain) learns through teaching; ANN can be taught and it can learn through training input-output data. After training, ANN can respond to unknown situation and has immense power to predict the possible output for new input data. ANN is specially suited to predict output where input-output relationship is not clearly known/understood; alloy properties in response to the constituent elements & its proportion is such a case.

For virtual metallurgy in ANN, the output nodes are the values of strength, hardness, toughness, ductility, etc. The input nodes may take values corresponding to % of the alloying elements but it has also to be decided that which & how many alloying elements have to be considered for the virtual alloy formation. Therefore a prep- procession to ANN is needed for proper input data selection. A post-processor may be needed to list the superior alloys [4-7].

II. ARTIFICIAL NEURAL NETWORK (ANN)

A. ANN Fundamentals

Artificial Neural Network (ANN) are often thought of as distinct from of artificial intelligence (AI). AI programs are based on logic & linguistics where as ANN programs simulate the biological process of human brain & nervous system. ANN are massively parallel processors that have a natural propensity for storing available experimental knowledge (experience) and making it available for future use (prediction) [8,9].

ANN (Considering 3 layered network), resembles the brain & woks in the following respects.

(i) Input data (signals) are fed to input layer neurons, say as: x_1, x_2, x_3, x_4.

(ii) The input to the intermediate–layer (hidden–layer) neurons, say at neurons 2 of the hidden layer as the weighted sum of x_1, x_2, x_3, x_4 i.e. equal to $w_{21}\, x_1 + w_{22}\, x_2 + w_{23}\, x_3 + w_{24}\, x_4$, where connecting links between the layers are called as synapses and the synaptic weights are $w_{21}, w_{22}, w_{23}, w_{24}$.

(iii) The weighted-input to the hidden layer neurons may activate or not-activate or partially activate the particular neuron depending on the layer activation function and threshold. The output of this particular hidden-layer neuron after activation function would become the input for the output layer neurons.

(iv) The input to a neuron of output-layer would be weighted sum of inputs to that neuron from the output-side of the hidden layer. The activation, once-again, of the output neuron will depend on activation function & threshold there.

(v) ANN can be taught from known data (past experience), usually it is called 'supervised learning'. From the known input-output data; input data is presented to the network and resulting output is compared with the target output and weights are adjusted in such a way to reduce the difference (error). This is done through an algorithm popularly/commonly known as 'back propagation algorithm' via forward pass and backward pass.

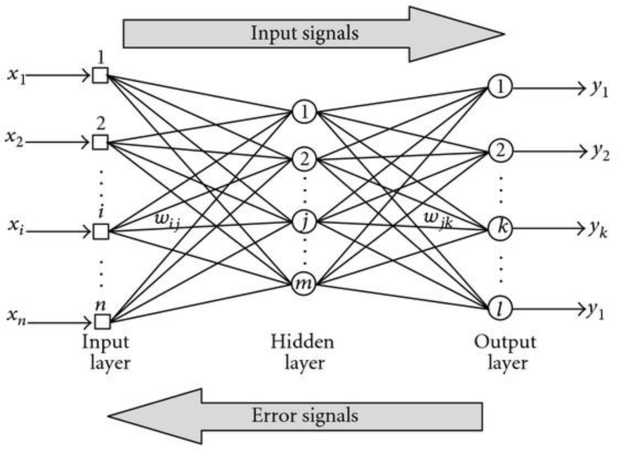

Fig.1. Schematic diagram of three layered back propagation neural network [18].

B. ANN Algorithm

A three layered feed forward back propagation algorithm, is simple, well known and used as described in Fig.1. Its fundamentals are described earlier. During 'forward pass' all the weights of the network are initialized randomly and the network output calculated, and the difference between the calculated and targeted output (i.e., error) are calculated (as described earlier). During/after the 'backward pass', the initialized weights are modified (adjusted) to minimize the error by propagating the error backwards. The network outputs and error are calculated again with the updated-weights, and the process repeats till the error in acceptably small. The two steps: forward pass and backward pass are described as [10-14]:

a) Forward Pass

The input training data to the network is (x_1, x_2, x_3, x_4). The net input to the hidden-layer neurons are

$$net_j^h = \sum_{i=1}^{n} \omega_{ji}^h x_i$$

wherein ω_{ji}^h represents the synaptic weight between the ith neuron of input-layer to j^{th} neuron of hidden- layer. The output y_j from the hidden-layer through activation function in given by

$$y_j^h = f_j^h \, (net_j^h)$$

wherein the activation/squash-function (sigmoidal) is

$$f(x) = \frac{1}{1+e^{-x}}$$

The net input to output layer at k^{th} neuron

$$net_k^o = \Sigma_{j=1}^{h} \omega_{kj}^o \; o_j^h$$

wherein ω_{kj}^o represents the synaptic weight between hidden & output layer, from j^{th} neuron of hidden-layer to k^{th} neuron of output-layer. The final output at the output-layer, through (applying) activation function (f), is given by

$$o_k^o = f_k^o \, (net_k^o)$$

The individual error (the difference between the target value Y_k and calculated value\$o_k$ at each output neuron unit $e_k^o = Y_k - o_k^o$ and the mean 'squared' error at all output unit E = $1/_2 \sum_{k=1}^{m} e_k^2$

b) Backward Pass

The weights between the output & hidden and between hidden & input layer are adjusted to minimize the mean square error in the backward pass. The adjustment, that is required in the weights are computed as

$$\Delta\, \omega_{kj}^o = \beta \; . \; y_j^h \; . \; e_k^o$$

$$\Delta\, \omega_{ji}^h = \beta \; . \; x_i \; . \sum (Y_k - o_k^o) . \; w_{kj}^o$$

For faster convergence, learning rate parameter β and momentum term α may be used; sometimes 'noise' addition could be beneficial for better learning.

c) Iterations

The process is repeated, till error is acceptably small. The weights are adjusted again & again with other sets of training data in similar way.

III. VIRTUAL METALLURGY

There are almost 103 known elements in periodic table with several isotopes and allotropy. Thus so many potential alloys of compounds could be thought of but its combinations/permutations that too with different % proportions are almost infinite. It is not easy/ feasible to physically, make and test properties experimentally, for all of these alloys/compounds. But on computer, it is possible to make these potential alloys or compounds and its properties prediction could be done through Artificial Neural Network algorithm. This novel concept of alloy formation and its properties prediction on computer is coined by the author as 'Virtual Metallurgy'. The Virtual Metallurgy is not limited to metallic alloys only, but in broader sense it is infact 'Virtual Chemistry', and includes compounds, **polymers**, ceramics and **composite materials**. However, since the present paper deals mainly with metallic-alloy formation and its properties prediction the name 'Virtual Metallurgy' is retained/ used.

A 3-layered feed forward back propagation **ANN** is used; the input data are % of alloying elements and the output neurons are the values of strength, hardness, ductility, toughness, corrosion resistance etc. as training data [15].

A. Alloy formation on Computer

The input data to the neurons of the input layer may take values corresponding to % of the allying elements but it has to be decided first that which & how many alloying elements are to be taken for the virtual formation of the alloy. For this a pre- processor to the **ANN** is needed for proper input data selection to form the alloy.

a) Alloy types-prepossessing

The author suggests 5 types alloy formation (pre-processing) (i) Universal alloys (ii) Grand alloys (iii) Classified alloys (iv) Mixed alloys (v) Other alloys.

(i) Universal alloys

Even if isotope and allotropy ignored, all the 103 elements are the 103 nodes of input layer, but if only few elements are taken into consideration other nodes may take zero values. This however, is a big exercise and may seem impracticable.

(ii) Grand alloys

Grand alloys may be of types (a) metallic alloy, (b) non - metallic alloy or (c) combination of both.

(a) For metallic type grand alloy all or many of the metallic elements such as Fe, Cu, Zn, Sh, Pb, Sb, Cr, Ni, W, Co, V, etc are the input nodes of input layer

(b) For non- metallic types grand alloy all or many of the non-metals such as C, Si, Ge etc and gases like oxygen (oxide), nitrogen (nitride) sulphur (sulphide) etc are the input. Example for this class is ceramic alloys.

(c) Combination type grand alloy is combination of (c) & (b) such as cermets.

(iii) Classified alloys

Classified alloy such as carbon steel (Fe+C), alloy steel (Fe+ other alloying elements), Brass (Cu+Zn), Bronze (Cu + Other elements), Duralumin (AI+Cu) etc. The classified alloy may be considered mainly as set of training data (as its composition & properties are known) for alloy formation of other categories.

(iv) Mixed alloys

Mixture of two or more types of classified alloys can yield a mixed alloy with better properties. In the present paper emphasis is given on a few mixed alloys and its properties prediction. If two classified alloys such as soft brass (Cu+Zn) and aluminium-bronze (Cu+AI) are mixed, for example, the input nodes are Cu, Zn & AI.

(v) Other alloys

Other alloys are the misc. alloys not covered in the above 4 categories of alloys. Such alloys could be **composites**. In broader sense considering 'Virtual Chemistry' it could be **polymers**.

b) Preprocessor for % proportion of the alloying elements

Once it is decided that which category of alloy is to be formed % proportion of the alloying elements are to be decided. For example, for mixed alloy as mentioned above (Cn+Zn+AI), first the range of these elements are to be decided from experience of common sense. Within these range, through a small computer program, various possible alloys are formed on computer by slightly (say1%) varying the % of these elements.

B. Alloy-Properties prediction of New Alloys through ANN

As described in the previous section, new alloys could be formed on computer by selecting the alloying elements and varying its proportion. In the present paper, however, only a few new 'mixed alloy' formation and its properties prediction are discussed. Two new categories of mixed alloys of potentially better properties are found as (i) (a) soft Braonze (b) hard Braonze (ii) Hc Hss tool material which are described below. Alloy - properties prediction could be made through ANN described earlier. Pre-processor generates a large variety of alloys and only few of them will be of improved quality/property. A post processor may be used to list the superior alloys.

a) Braonze

Braonze is a new mixed alloy which can be thought of as mixture of brass (Cu+Zn) and bronze say aluminum-bronze (Du+AI) and thus named as Braonze. The 3 input nodes are Cu, Zn & Alone hidden layer with two nodes are taken. Two sets of training data are corresponding to the classified alloys of brass & bronze are available i.e., composition of brass and bronze and its properties are already known. Using the training data to the three layered (3-2-2 neurons) feed forward back propagation ANN, the ANN could be trained (i.e. weights are adjusted). Varying the % of Cu, Zn & AI of the new mixed alloys (Le Braonze) to the trained ANN, it can be found that which of these Braonzes are superior over its constituent classified alloys (brass & Bronze). Superiority of the new mixed alloy could be ensured be increasing the threshold values of the 2 output nodes corresponding to softness (% ductility) and hardness (BHN).

It is found that the two new mixed alloy namely soft-Braonze (65% Cu, 30% Zn, 50% AI) and hard-bronze (55% Cu, 40% Zn, 5% AI) have improved properties. The soft-braonze is softer than soft-brass and aluminum-bronze where hard braonze is much harder than hard brass. So Braonze is not only having good properties of brass and bronze but its range for softness of hardness is widened than that available within brass & bronze.

The Braonze so discussed are infact AI-Braonze. Sn-Bronze with brass can yield Sn-Braonze, Ni-Braonze with brass can yield Ni-Braonze & so on. Infact, German silver (60% Cu, 20% Zn, 20% Ni) can be called as Ni Braonze & Gun Metal (88% Cu 10% Sn, 2% Zn) can be called as Sn Braonze. So it is possible to find a whole range of Braonzes with possible improved properties.

b) Hc- Hss tool material

Hc-Hss is a new mixed alloy which can be thought of as mixture of High carbon steel and High Speed and thus named as Hc Hss tool material. The 5 input nodes are % Fe, C, W, Cr, V. Two sets of training data are corresponding to the classified alloy of high carbon steel and high spread steel are available Le. Composition of these and its properties are known. Using the training data to the 3 layered (5-2 -2 neurons ANN), the ANN could be trained (weights adjusted). Varying the % Fe, C, W. Cr, V, different possible alloys could be formed on computer. Feeding % of the alloy elements to ANN it can be found which of the alloys have better properties than its constituent classified alloys. Superiority can be ascertained of increasing the value at the 2 output nodes corresponding to toughness (say % ductility x strength) and hardness (BHN) through post processor.

It is found that a new mixed alloy namely HcHss (76% Fe, 1% C, 18% W, 4% Cr, 1% v) is having improved property. It has higher can hardness than high speed steel so possibly higher hot hardness than high speed steel.

c) Other possible mixed alloys

In a similar pattern/technique used for Braonze and HcHss as explained earlier, other possible mixed alloy could also, be found. Author suggests a few potential mixed alloys as follows. Brass- steel (Fe+C+Cu+Zn) could be thought of as mixture of mild steel and brass, which should have proportion of mild steel as well corrosion resistance due to Zn & Cu. Aluminum-steel, (Fe, C, AI) could be thought of as mixture of aluminium and mild steel, which should be a lighter steel. Several such permutations / combinations could be tried upon through virtual metallurgy and it is expected to get many news alloys of interesting & improved properties.

IV. VIRTUAL - CHEMISTRY AS BROADER SENSE OF VIRTUAL - METALLURGY

'Virtual-Metallurgy', in broader sense is infact 'Virtual-chemistry', and thus can find applications for formation and properties prediction of 'new' chemical compounds & drugs, 'improved' plastic, 'quality' ceramics and 'better' composite materials etc.

For new chemical compounds & drugs, the input modes would be the chemical elements and the output nodes would be its physical/ chemical & medicinal properties. The training data could be taken from the known compounds 4 drugs. Care should, however, be taken that whether new compounds & drugs are chemically feasible or not.

For improved polymer plastics, the input nodes may be taken items such as monomers, binder, cross-link agents etc and the output nodes would be its properties. Training data may be taken from known **polymers**.

For quality ceramics (Say for production of quality glass), the output quality (such as transparency) depends on the ingredients of inputs (such as type & proportion of sand, temperature & process); so it is possible to find new quality ceramics. Training data may be taken from known ceramics. Also as described earlier, new high Te superconductors could be found.

For better **composite materials**, the input nodes may be taken as items such as fiber, of combination of fibre, matrix material, and process etc and the output nodes would be its properties, training data may be taken from known **composite materials**.

The applications of virtual-metallurgy/ virtual chemistry are endless. Some research workers have been using [16] in a way this concept without referring it (because the systematic & rigorous introduction of virtual metallurgy/ virtual-chemistry has been made in the present paper and the name virtual metallurgy/ virtual chemistry is coined by the author [17].

The future of virtual-metallurgy (which encompasses virtual-chemistry and virtual-testing too) seems to be very bright.

V. CONCLUSIONS

The novel concept of 'virtual-metallurgy' for alloy formation and alloy properties prediction through 'Artificial Neural Network' on computer is successful and have high potential for wide ranging applications.

Few new alloys of improved properties are found and reported several other wide ranging applications are suggested.

Virtual-metallurgy in broader sense is virtual-chemistry and would gain its popularity in due course, and would become indispensable tool for metallurgists & chemists in the 21st century. Its importance as eco-friendly metallurgical manufacturing for sustainable development will be more evident.

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