

Application of artificial intelligence to modeling of materials performance and processing

D. SANYAL

National Metallurgical Laboratory, Jamshedpur - 831 007, India.

ABSTRACT

This paper reviews the state-of-the-art in artificial intelligence research pertinent to metallurgical and materials science. The frameworks of two broad schools of AI research, namely, the Expert Systems (ES) and Artificial Neural Network (ANN) have been discussed with specific reference to their various notable applications in the area of materials research. Finally, we present NML's own efforts in this area, where a hybrid framework comprising ES and ANN is being developed for future use.

INTRODUCTION

The term, Artificial Intelligence (AI) - as generally believed - was first introduced by John McCarthy in a conference at Dartmouth College at Hanover, New Hampshire in USA way back in 1956. In principle, the name owes its origin to an effort to mimic the learning process of a human being by associating logic to infer rules or "pattern" from a closely connected phenomena or facts. This mimicking has been sought through the use of a combination of computer based techniques and the mathematical framework of knowledge representation (such as, predicate calculus, production systems etc.) and a logic of uncertain reasoning, named the fuzzy logic. AI has come long way since then and has gradually gained recognition among knowledge - intensive professions, such as, medicine, chemistry geology, social sciences, economics and certain domains of engineering where diagnosis and design are ruled more by heuristics than by mathematical formulae. AI means many things to many persons - starting from knowledge-based systems to speech recognition, robotics, computer vision and so on. In the present context of materials research, we shall narrow our scope to define AI as a broad framework within which two predominant techniques, namely, Expert System (ES) and Artificial Neural Network

(ANN) have recently made significant impact.

EXPERT SYSTEM

Expert systems are computer programs which are endowed with human like features of intelligence, namely, knowledge, skill, reasoning and learning. Unlike conventional number-crunchers, the expert systems do not run step-by-step procedures and algorithms to solve a problem. (They are the so-called "intelligent" systems which emulate the way humans employ past experience and available information to solve new problems heuristically.) The components of an expert system are four basic modules :-

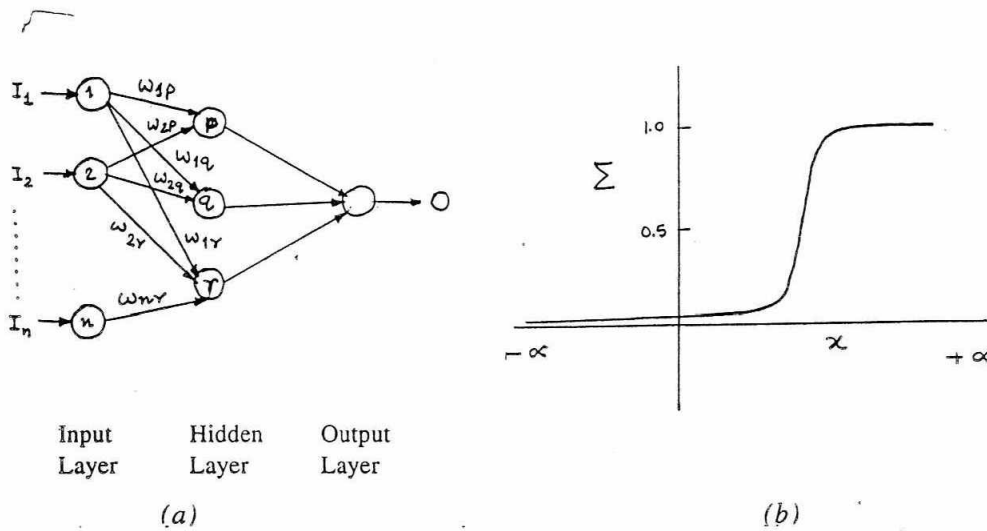
- i) a knowledge base comprising facts (data in handbooks and form experiments) and rules (heuristic rules of thumb about a specific domain)
- ii) an inference mechanism which performs
 - inductive or deductive reasoning to draw logical conclusions from facts and rules
 - resolves conflicts between inconsistent facts or goals.
- iii) a knowledge acquisition tool which imparts ability of the system to "learn" by updating its knowledge base and
- iv) a natural language processing interface which provides the user a friendly window to communicate to the system.

The ES are distinctly different from traditional simulation programs on the following counts :

- a) conventional softwares represent and manipulate data, whereas Expert Systems represent and manipulate knowledge.
- b) conventional softwares can use only algorithms, but Expert Systems can use both algorithms and heuristics
- c) conventional softwares rely on repetitive processes, but Expert Systems use inferential processes
- d) conventional softwares are like "opaque black-boxes" which do not reveal their algorithm to the user. Expert Systems use transparent reasoning and displays, on request, its line of reasoning to the user.

In highly complex systems where the domain knowledge is, in prin-

inciple, too fuzzy to allow a quantitative description, ES is likely to provide more reasonable qualitative or semi-quantitative solution. The domain of materials and metallurgical engineering undoubtedly belongs to the category of qualitative systems as the complexities and non-linearities of each process or phenomena are too many - thus defying precise quantifiability in terms of a mathematical or even semi-empirical framework. We shall shortly illustrate this point with a few areas of materials research, namely, material design and failure analysis.



(a) (b)
 Fig. 1:(a) Schematic of feed-forward multilayer ANN,
 (b) Sigmoidal activation function

Expert System in Material Research - State-of-the-art

Since the first ES, DENDRAL was successfully developed at Stanford University in 1965 to aid organic chemists in determining molecular structure of compounds, a host of expert systems have been built and found applications in medicine, chemistry, bioengineering, electronics, computer systems and military. Over the last couple of decades, ES applications to materials evaluation, design and processing have been noticed. The most notable advances have been made in Japan. The most well known among them is NKK-BAISYS an expert system developed for the 10000 tonnes per day blast furnace No. 5 of the Fukuyama Works^[2]. The tasks performed by the above are twofold - (a) abnormal condition diagnosis that predicts the risk of burden slipping and channelling and suggest countermeasures (b) furnace heat level control that determines the current level of furnace heat, forecast

how it will change, suggests and executes proper actions. A detailed review of other expert systems for BF operations at Sumitomo Metal Industries, Kawasaki Steel Corpn. and Nippon Steel as well in Nordic countries is given in ^[3]. The advantage of ES in iron and steelmaking reported so far are impressive. An ES, installed in a steel plant, reportedly plans steelmaking schedules, thereby cutting scheduling time from 3 hours to approximately 30 minutes, reducing refractory costs and increasing the efficiency of the equipment ^[4]. Another steelmaking plant is using a diagnostic ES to improve productivity and quality. An additional benefit is the preservation of the knowledge of the plant's experts. It has been claimed ^[5] that the system has already produced enough savings, virtually paying for the entire development program in a single year. The ES of Nippon steel was reported to have a 98% hit rate (i.e. 98% of the suggestions made by this system to the furnace operators were found worthwhile for implementation) by continuous maintenance and development of more than 5000 rule ^[3]. ES has been assisting in hierarchical control schemes. Apelian and Meystel presented a general structure of a knowledge-based controller^[6]. Subsequently, computer control packages featuring ES have been implemented in cold rolling mill, welding inspection and LD operations ^[7,8,9].

Apart from iron and steelmaking processes, expert systems are also being used for alloy design ^[10], failure analysis ^[11], life prediction ^[12], heat treatment ^[13], materials synthesis ^[14], thermodynamics ^[15], metal forming ^[16], alloy melting and son on ^[17]. More recently, it has been shown that expert systems can control ferroalloy processes ^[18]. Several detailed reviews of applications of ES to the materials and metallurgical engineering can be referred for further reading ^[19].

ARTIFICIAL NEURAL NETWORK

If expert systems could be classified as "qualitative" intelligent systems, neural networks fall in the category of "quantitative" artificial intelligence techniques. Artificial Neural Networks, as the nomenclature suggests, are computational methods that loosely mimics the way the human brain functions through interconnected biological neurons in recognising "patterns". The ANNs comprise computational nodes, known as, neurons or perceptrons which are connected by links. Each of the neurons - the basic cell of the network - has some inputs (I_1, I_2, \dots, I_n) and one output (O) (Fig. 1a). Each input value i_j is multiplied by a weight w_j . The sum of all these products is converted by a suitable transfer function Σ which is usually sigmoidal in nature

defined in the interval $-1 < \Sigma < 1$ and gives the nodal output. The network is usually a multilayer structure of neurons where the output O of a neuron is weighted and input to the next layer. Nodes of the same layer do not communicate to each other. Inputs to neurons of the first layer corresponds to network inputs and outputs from the last layer are the network output. The large number of neurons and their complex interconnections give the ANN brain like functionality of "learning" patterns. The learning process of ANN is performed with a "training" algorithm. The network is fed with a large number of examples representative of the task to be accomplished by the network, known as, "patterns". Each example has input vector $I(I_1, I_2, \dots, I_n)$ and output vector $O(O_1, O_2, \dots, O_m)$. The training starts with a set of randomised weights for the links in the ANN. The computed outputs from the network $T(T_1, T_2, \dots, T_m)$ are then compared with the output vector O and the sum squared error is minimised by modifying the weights of connections between intermediate level units in an iterative cycle through an appropriate algorithm, such as, the backpropagation algorithm ^[20]. Once the training is complete, ANN can predict output behaviour for a new set of patterns.

Apart from the above function of pattern-association based on the multilayer back-propagation algorithm, an ANN can perform pattern classification, self-organisation, pattern mapping, signal analysis, fault diagnosis, noise filtering, spatio-temporal system simulation and optimisation, based on alternate formalisms, such as, the Hopfield network ^[21], the extended learning vector quantization network ^[22], spatio-temporal pattern recognition network ^[23], general associative network ^[24], brain-state-in-a-box ^[25], self organising map network ^[26], probabilist neural network ^[27] etc.

The salient differences of ANN with traditional modelling and computational approaches are :

- i) ANN performs computations without mathematical model of system by propagating changes in activation between the neurons
- ii) ANN is able to self-organise, learn and classify patterns from a mass of input/output data
- iii) ANN can work with incomplete, partially correct, noisy or uncertain (fuzzy) "patterns" or data set and produce correct or nearly correct response.

- iv) ANN can generalize rules from the cases on which they are trained and apply these rules to new patterns.

Artificial Neural Network in Materials Research

Since the publication of Rumelhart's seminal work on ANN [20], ANN has become the fastest growing discipline within AI over a decade's time. Apart from the computer scientists, electrical and chemical engineers have fiercely engaged themselves in ANN research [21 to 33]. Despite its tremendous advantages, use of ANN in materials research is still a minuscule portion of the total body of ANN literature. This may be attributed to the inability of the materials scientists and metallurgical engineers to learn from the advancements of other disciplines. Some applications of ANN in the domain of materials research is summarised below.

Kortesis and Panagiotopoulos [34] have formulated and solved static structural analysis problems in a neural network. The crux of their effort was to solve an inverse problem for unilateral and bilateral structures - that is, to estimate the elastic properties and/or loading and/or geometric quantities which will supply a solution very close or identical to the prescribed one. Employing a Hopfield-like neural model [35], they obtained very good agreement between the estimated modulus of elasticity and Poisson's ratio ($E=2.495 \times 10^6$ t/m², $\nu=0.28$) and the known solution ($E=2.5 \times 10^6$, $\nu=0.30$).

Onda *et.al.* [36] of Komatsu Limited, Japan have used an ANN for weld defect identification. As part of their Computer Integrated Manufacturing (CIM), a programme was launched to automate the ultrasonic inspection of welding defects. The need for evolving such a system was felt because of several drawbacks of the erstwhile manned inspection system. The test piece was a V-Weld of two 16mm thick plates, set 5mm apart and welded to a back plate by CO₂ arc. The four defect types to be inspected were remaining root and defective fusion, cracking, slag inclusion and pinhole. The ANN were trained with 384 test patterns from a defect distribution diagram on an ultrasonic display tester comprising defect distribution on horizontal section and lengths of defects on weld section. The recognition accuracy of the ANN was 80% and the average defect identification rate was 75%, which was nearly the same as that achieved by expert engineers.

Reuter and van Deventer [37,38] applied ANN to derive kinetic rate

equations for identification of the process conditions and dynamic simulation of batch and continuous metallurgical and mineral processing systems. Reactor identification implies by what degree the conditions within the reactor, i.e. reagent levels, pH, pulp density, temperature, pressure etc. change the kinetics of the process. The ANN was applied for training data sets of :

- i) industrial zinc hydrometallurgy, namely, the leaching of a Zn ore and the precipitation of Fe^{3+} ions from Zn-leach liquors
- ii) a flotation rougher circuit for the recovery of copper sulphide
- iii) reaction fault diagnosis in the flotation circuit as above.

The ANN was able to learn in all cases the training data set within acceptable error limits.

Reisener *et.al.*^[39] have used ANN for studying mass transfer in gas-sparged electrolyzers. Reuter *et.al.*^[40] have used ANN for modelling slag-metal equilibrium processes in pyrometallurgical reactors.

APPLICATIONS OF ARTIFICIAL INTELLIGENCE IN INDIA

In the Indian context, AI as a tool, has been confined to academic research and found limited practical application. This is as much due to a lack of awareness in the industry of its strength as to the lack of efforts from the R&D and academia to bridge existing communication gaps. Moreover, AI is perceived as a threat to employed human resources instead of an aid. It is therefore not surprising to find very few efforts made in India to develop and apply ES.

In management of natural resources, such as geographic information systems, land use/land cover, soil classification, image analysis etc. several Indian efforts have been noted^[41]. In the area of metallurgical systems, Kumar *et.al.* have developed an ES for steel annealing, Venkateswarlu and Gangiah have used signed directed graph and fuzzy logic for fault diagnosis of titanium dioxide kilns, Satyanarayana *et.al.* have developed a prototype ES for the autonomous process operation of a titanium sponge production plant and Palani *et.al.* have developed an ES for welding of stainless steels^[42]. Varkey has developed a self-learning automation in steel plants using operator knowledge embedded in an ES and Nair and John have developed an ES for maintenance of rolling mills^[43]. Not much effort has been noted till date in the

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development and application of ANN for metallurgical industries.

At the computer applications division of National Metallurgical Laboratory (NML), Jamshedpur, an Expert System shell "CONSULT" has been developed in Turbo-PROLOG with features of knowledge representation using IF-THEN rules, knowledge acquisition, data representation and natural language interface to the user. A small prototype expert system has been built and tested for thermodynamic analysis of vapour-liquid equilibria. In principle this ES shell is general purpose and can be adapted to develop expert systems in other applications, such as alloy design ^[44], failure analysis etc.

An ANN software is under development. A prototype ANN based on multi-layer backpropagation rule has already been built and applied to modelling of a BOF steelmaking process ^[45]. Advanced features, such as genetic algorithm and fuzzy logic have been provided in the ANN model. Refinements and testing of the model are underway.

The powerful RISC based HP 9000/75 CAD Workstation at NML with 135 MIPS, 40 MFLOPS and high resolution graphics will be useful for ANN softwares of moderate size which is typically generated for modelling a metallurgical system.

CONCLUSION

The status of AI application in metals and materials science and engineers has been briefly reviewed in this paper. It has been shown that AI is not only emerging as a promising field for the computers scientists, but bear great future for materials research. Owing to the intuitive and semi-empirical nature of knowledge base involved in materials design and processing, an ES-ANN hybrid route of modelling might emerge as the most suitable framework in future work has already been initiated at NML in that direction.

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