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EXPLOITATION OF NEURAL NETWORKS IN MATERIAL RESEARCH

VYUŽITÍ NEURONOVÝCH SÍTÍ V MATERIÁLOVÉM VÝZKUMU

Abstract

Theoretical knowledge of physical metallurgy doesn't express comprehensively all physical variables, which influence resultant product manufacture quality. Therefore data files contained in IRA and ARA steel diagrams of different chemical composition are the basic tool for heat treatment. It is possible to treat these data statistically and thus acquire empiric relations, which serve for partial processes course prediction proceeding at heat treatment. These relations were obtained so far on the basis of regression analysis of measured data. Real possibility of prediction of different steel parameter with exploitation of artificial intelligence elements offers at present. Model of prediction steel mechanical properties after heat treatment using neural networks methods were created. The problem is solved in the framework of the grant project GAČR 106/05/2596.

Abstrakt

Teoretické poznatky fyzikální metalurgie nepostihují dosud komplexně všechny fyzikální proměnné, které ovlivňují výsledné mechanické vlastnosti výrobku. Proto jsou základní pomůckou pro tepelné zpracování IRA a ARA diagramy oceli o daném chemickém složení. Údaje obsažené v IRA a ARA diagramech je možno statisticky zpracovat a takto dojít k empirickým vztahům, které slouží pro predikci průběhu dílčích procesů probíhajících při tepelném zpracování. Doposud byly tyto vztahy získávány na základě regresní analýzy naměřených dat. V současné době se naskýtá reálná možnost predikce různých parametrů oceli při tepelném zpracování s využitím prvků umělé inteligence. Byl vytvořen neuronový model pro predikci mechanických vlastností ocelí po tepelném zpracování. Daná problematika byla řešena v rámci grantového projektu GAČR 106/05/2596.

1 INTRODUCTION

One of the fields, where it is possible to exploit neural networks, there is a prediction of mechanical properties of materials on the basis of their composition and preceding treatment. Final steel product manufacture properties of given size and form depend on its chemical composition, on steel technology, type of semi product, forming and heat treatment technology. Steel and forming technology have a considerable importance from the steel products final properties point of view, because together with chemical composition and so-called steel purity (influence of basic raw materials) they create the basis of properties of these materials. These properties however can be partially influenced by a heat treatment. Inappropriately selected or executed heat treatment technology thus can be also the cause that manufacture properties of steel products are not achieved.

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Theoretical knowledge of physical metallurgy does not express comprehensively all physical variables, which influence resultant product manufacture quality. Therefore data files contained in IRA and ARA steel diagrams of a different chemical composition are the basic tool for heat treatment. It is possible to treat these data statistically and thus acquire empiric relations, which serve for prediction of course of partial processes proceeding at heat treatment. These relations were obtained so far on the basis of regression analysis of measured data. A real possibility of prediction of different steel parameter with exploitation of artificial intelligence elements offers at present.

The aim of the paper is to outline possibilities of artificial neural networks application for prediction of mechanical steel properties after heat treatment and judge perspectives of their exploitation in this field.

2 NEURAL NETWORK DESIGN AND OPTIMIZATION

Neural networks use a distributed parallel processing of the information during practising the calculations, it means that information recording, processing and transferring are carried out by means of the whole neural network then by means of particular memory places. Learning is a basic and essential feature of neural networks. Knowledge is recorded especially through strength of linkages between particular neurons. Linkages between neurons leading to "correct answer" are strengthened and linkages leading to "wrong answer" are weakened by means of repeated exposure of examples describing the problem area. These examples create so called training set.

A capability to learn from examples and to describe non-linear dependences is a big advantage of neural networks. A disadvantage is the fact, that a size of error, which is dependent on network parameters and on a training set, cannot be generally estimated in advance. The design of a structure and parameters of the neural network is always connected with some experiences. The experience, intuition and experiments are also important for the optimization of the neural network. Neural networks, which are universal function approximators, consequently especially networks utilizing for their learning Backpropagation algorithm, are suitable essentially for all types of predictions. This algorithm is suitable for multilayer feedforward networks learning, which are created minimally by three layers of neurons: input, output and at least one inner (hidden) layer (Fig. 1). Between two adjoining layers there is always so called total connection of neurons, thus each neuron of the lower layer is connected to all neurons of the higher layer. Learning in the neural network is realized by

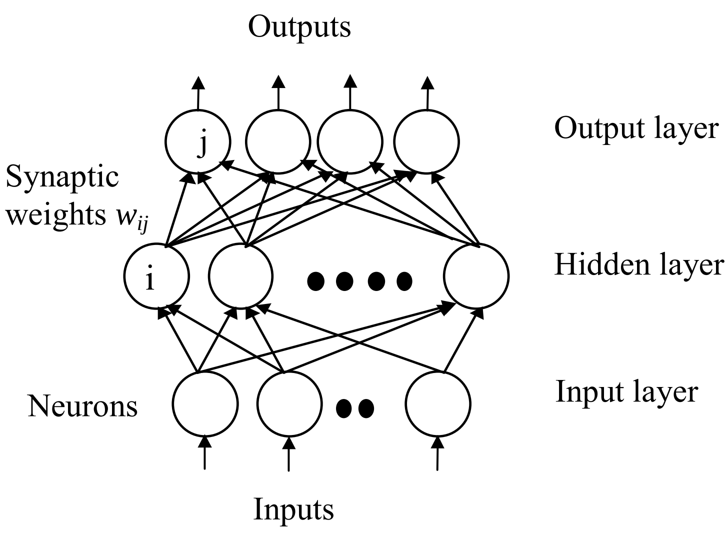

Fig. 1 Topology of multilayer feedforward neural network

setting the values of synaptic weights between neurons, biases or inclines of activation functions of neurons. The adaptation at Backpropagation types of networks calls „supervised learning“, when the neural network learns by a comparison of the actual and the required output and by setting values of the synaptic weights (biases or inclines), so that a difference between the actual and the required output decreases.

The rate of inaccuracy between predicated and actual output represent a prediction error. In technical applications the error is mainly represented by following relations [3]:

- relation for RMS error calculation (Root Mean Squared) – it does not compensate used units

$$RMS = \sqrt{\frac{\sum_{i=0}^{i=n-1}(y_i - o_i)^2}{n-1}} \tag{1}$$

- relation for REL_RMS error calculation – it compensates used units

$$REL\_RMS = \sqrt{\frac{\sum_{i=0}^{i=n-1}(y_i - o_i)^2}{\sum_{i=0}^{i=n-1}(y_i)^2}} \tag{2}$$

where: n - number of patterns of training or test set, y_i - predicted outputs, o_i - measured outputs.

3 PREDICTION OF MECHANICAL PROPERTIES OF STEEL AFTER HEAT TREATMENT

In the field of research oriented on metallurgical technologies control with the aim to optimize the industrial process and to increase a quality of materials by application of artificial intelligence elements particular models of artificial multilayer neural networks for prediction of material mechanical properties after heat treatment were designed and gradually tested.

These models predicted final mechanical properties as tensile strength (R_m), yield strength (R_e), elongation (A) and area reduction (Z) of material on the basis of knowledge of chemical steel composition and conditions of heat treatment. For learning and for verification of neural networks functionality data from catalogue of experimental heats were used [2]. Content of 10 elements of chemical composition of steel and 6 possible resultant structures represented by a different cooling rate and drawing temperature are stated for each heat.

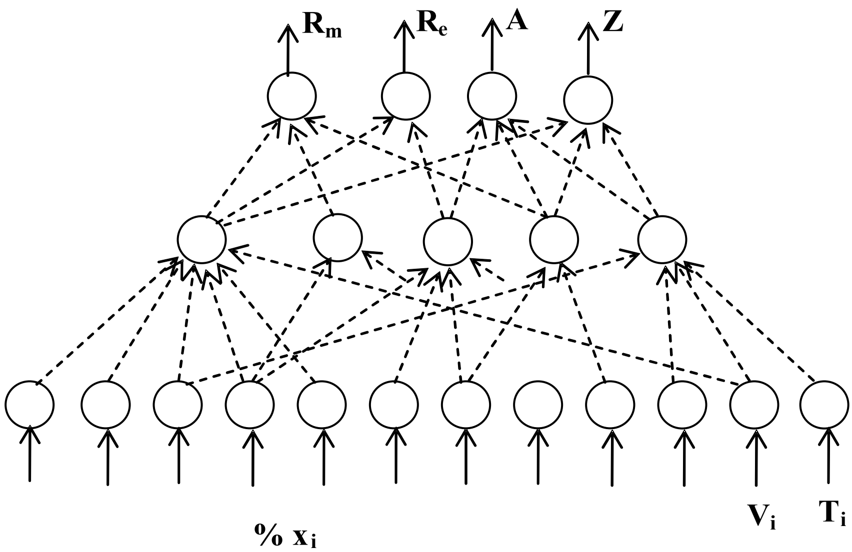

Fig. 2 Multilayer feedforward neural network

Austenitizing temperature and dwell time upon this temperature were at all heats the same: 880 °C for a period of 1 hour. All heats have also the same drawing time: 8 hours. Therefore these parameters were not included into the neural network inputs. The whole catalogue is divided into the two groups: the first group contains constructional steels grade 12 – 16 determinate for hardening treatment, the second group Cr- Ni- Mo steels with content 0,2-0,6 %C (carburizing, rotor, tool steels). A neural network, which output layer was created by 4 neurons, was designed (Fig. 2). Neuron outputs represented mechanical properties of steel: tensile strength (R_m), yield strength (R_e), elongation (A) and area reduction (Z). Input layer was created by 12 neurons. Their values represented basic parameters, which had influence to predicted mechanical properties value: 10 elements of chemical steel composition, cooling rate and drawing temperature. Total number of patterns used for neural network learning was 273 and remaining 45 patterns served as a testing set.

It was possible to distinguish two separated groups in analyzed heats according to their chemical composition. The first group created constructional steels grade 12 – 16 determinate for hardening treatment (below marked as „normal steels”) and the second group steels grade 16 (carburizing and rotor steels) and steels grade 19 (tool steels) with higher content of Cr, Ni, Mo and V (below marked as „alloyed steels”). These groups markedly distinguished in resultant mechanical properties. The neural network modeling was performed using MATLAB - Neural Network Toolbox software. For particular neural network models a quality of network adaptation to the submitted patterns and generalization scale were observed.

The best results of mechanical properties prediction proved neural network models, which topology and prediction errors RMS and REL_RMS calculated according to relations (1) a (2) are showed in tables 1 a 2:

Tab 1. RMS error for selected network topologies

Steels	Topology	RMS			
		R_e	R_m	A	Z
		[MPa]		[%]	
Normal and alloyed	12-3-5-4	82.73	62.40	1.67	4.1
Only normal	12-3-4	33.07	36.25	1.44	4.9
Only alloyed	12-3-3-4	98.70	61.96	1.45	4.8

Tab 2. REL_RMS error for selected network topologies

Steels	Topology	REL_RMS			
		R_e	R_m	A	Z
		[MPa]		[%]	
Normal and alloyed	12-3-5-4	0.099	0.065	0.083	0.064
Only normal	12-3-4	0.036	0.047	0.066	0.079
Only alloyed	12-3-3-4	0.107	0.059	0.076	0.075

Suggested network was able to satisfactorily predicate mechanical properties of constructional steels grade 12 – 16 determinate for hardening treatment with average error at particular properties up to 7,5 %. Prediction results of steels grade 16 containing Cr, Ni, Mo, V and grade 19 were in results little worse. Average error at prediction of particular properties was at the most 8,2 %. However these heats were represented in training set by a less number of patterns.

3 CONCLUSIONS

Different mechanisms have influence to final mechanical properties of steels, which are moreover in mutual interaction: phase transformation, grain size, precipitates and dislocations. All these factors bring into processes strong non-linearity and dependences of superior degrees and very complicate accurate models creation. After evaluation of results we can state that exploitation of neural networks is advantageous, if it is necessary to express complex mutual relations among sensor-based data and thus also at prediction of mechanical properties of steels.

REFERENCES

[1] JANČÍKOVÁ, Z. & VROŽINA, M. & SROVNAL, V. Utilization of neural networks for steel thermal treatment modeling, In *Simulation, Designing and Control of Foundry process FOCOMP '99*, Poland, Krakow, 1999, pp.159-164, ISBN 83-911283-1-8.

[2] Katalog výsledků charakteristik základních řad konstrukčních ocelí tř. 12-16 a ocelí tř. 19 po tepelném zpracování, Škoda – ÚVZÚ, Plzeň, 1986

[3] MYLLYKOSKI, P. & LARKIOLA, J. & NYLANDER, J. Development of prediction for mechanical properties of batch annealed thin steel strip by using artificial neural network modeling, *Journal of Materials Processing Technology*, No. 1-4, Vol. 60, 1996, pp. 399-404

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