Kohonen Network Modelling for the Strength of Thermomechanically Processed HSLA Steel

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Primarily from the point of view of improvement of yield strength due to additions of niobium, titanium and boron in HSLA steels, the experimental steels are divided into five classes. The data are then supplied for learning a Self Organising Map (Kohonen network). It is found that the network with six neurons possesses better capacity of prediction with unknown data. Another effort of clustering the steels according to its major strength contributing mechanisms is also made. But the capacity of the network to cluster unknown data is found to be rather poor and has failed to follow from the metallurgical principles. To avoid this limitation, Learning Vector Quantisation method is adopted to impart a certain amount of supervision in the learning process and it is found that the training pattern of the network attains a good convergence thereby leading to a good predictive ability.

KEY WORDS: thermomechanical processing; HSLA steel; yield strength; self organising map; Kohonen network; learning vector quantisation.

1. Introduction

In high strength low alloy (HSLA) steels thermomechanical controlled processing (TMCP) is a widely used process. To achieve the required microstructure and mechanical properties of a thermomechanically processed HSLA steels it is necessary to have knowledge about the role of composition and process parameters. The chemistry of the steel and the TMCP parameters, like reheating temperature, amount of deformation in different stages of rolling, the finish rolling temperature and the cooling rate are known to exert appreciable influence on the structure and property of the finished product. But all these inputs are related to the six basic strengthening mechanisms viz. precipitation hardening, grain refinement, microstructures, solid solution hardening, dislocation hardening and texture hardening, which ultimately govern the final properties of the steel.

Artificial neural network (ANN) is a kind of intelligent system, which tries to map the existing input output relationship in a much more accurate way.\(^1\) Used with back propagation algorithm, this technique has been found to be quite useful in predicting the mechanical properties, which depend on large number of independent input variables.\(^2 \text{--} 4\) Efforts have been already made to model the mechanical properties including the tensile strength, yield strength and percentage elongation of thermomechanically processed HSLA steels through conventional feed forward neural network with supervised back propagation algorithm\(^5\) and with Petri neural network.\(^6\) In this work modeling of similar system has been done through the Self Organising Map (SOM) or Kohonen network,\(^7\) which uses unsupervised learning of the neural network. Further, Learning Vector Quantisation (LVQ), a method for training competitive layers in somewhat supervised manner, has been used to separate the datasets comprising of composition and process parameters of the thermomechanically processed HSLA steel in accordance with the dominant strengthening mechanisms operative on the steel due to its particularity in the stoichiometry and processing variables. As knowledge plays an important role in the reasoning process of an intelligent system for solving real world problems and expressions of a knowledgebase are generally uncertain and are not free from human error and bias, reasoning under such circumstances often yields inaccurate measure in the inferences. Automatic estimation by unsupervised learning technique can be used in some of such cases to overcome this factor of uncertainty. This type of network has been successfully applied for Well Log calibration in the field of Petroleum Geology.\(^11\) But in the field of Materials Science its application is still insignificant.

2. Modelling Techniques

2.1. Self Organising Map

The Self Organizing Map or Kohonen network has a single layer of units and during training, clusters of units become related with different classes (with statistically similar properties) that are present in the training data. The Kohonen network is useful in applications where it is important to analyse a large number of examples and identify groups with similar features. It is an algorithm used to envisage and interpret large high dimensional data sets by projecting them on to a low dimensional space that has typ-
Fig. 2. The architecture of a learning vector quantisation network.

classify input vectors in much the same way as the competitive layers. The linear layer transforms the competitive layer’s classes into target classifications defined by the user. The classes learned by the competitive layer are referred as subclasses and the classes of the linear layer as target classes.

Both the competitive and linear layers have one neuron per (sub or target) class. Thus, the competitive layer can learn up to $S_1$ subclasses. These are combined by the linear layer to form $S_2$ target classes ($S_1$ is always larger than $S_2$).

3. Database

The data used for the present exercise have been mostly generated in the laboratories. The alloys have been prepared in laboratory-scale induction melting furnace and the chemical analyses are done in atomic spectrometer. The alloys in hot forged condition with thickness of 12.5 mm were heated to various temperatures within 1 000–1 250°C for 30 min and subjected to controlled rolling in a laboratory scale two high rolling mill. Three different types of cooling rate viz. water quenching, oil quenching and air-cooling were employed for the steel after different amount of deformation in different temperature ranges. The mechanical testing has been carried out in INSTRON 4204 machine with tensile specimen conforming to ASTM specification. The yield strength values calculated from the stress–strain curves were used for this particular work and referred as strength in all the cases. Some data from the published literatures are also taken into consideration for getting a wide range of variables.

4. The SOM Models

4.1. Effects of Niobium–Titanium–Boron on Strength

It has been found by earlier workers that if boron is added in combination with niobium, a remarkable improvement in strength can be achieved. It is also reported that the presence of niobium and boron in combination retards the recrystallisation of grains during TMCP and exerts a synergistic effect. This is credited to the non-equilibrium segregation of boron at dislocations and to the formation of Nb–B complexes. Addition of Ti with B has almost indistinguishable effect; however the grain refinement is comparatively less significant than the steel with niobium and boron. From the point of view of strength improvement due
to these additions, the HSLA steels of same basic composition and having niobium, titanium and boron, either singly or in combination, with similar basic composition, can be divided into five classes:

i) Steel with niobium
ii) Steel with titanium
iii) Steel with niobium and boron
iv) Steel with titanium and boron
v) Steel with niobium, titanium and boron

The data supplied to the SOM model is plotted as training vectors in Fig. 3 according to their initial mapping in the input space. The five different clusters are clearly visible in this map. Initially, four neurons are used to cluster these data. Before the beginning of the learning process, the initial neurons are all concentrated at the centre (the black spot in Fig. 4). After learning the network with 5 000 epochs, the weight vectors of the neurons are found to be distributed in the manner shown in Fig. 5. Similar learning is repeated with 6 and 8 neurons (Figs. 6 and 7). It is found that the network with six neurons possesses better capacity of prediction with unknown data. The input weights connected to the neurons are plotted in Fig. 8 to get an idea of the assigned weightages of the three alloying elements in case of different clusters.
4.2. Identification of the Dominant Strengthening Mechanism

It is well known that the alloying elements as well as the process parameters contribute to the mechanical properties of the thermomechanically processed HSLA steel through six definite mechanisms, viz. precipitation hardening, grain refinement, microstructures, solid solution hardening, dislocation hardening and texture hardening.

Nb and Ti are known to improve the strength through precipitation hardening, grain refinement and microstructural modifications, as discussed before. These effects are enhanced when those microalloying elements are added in combination with B. Copper strengthens the HSLA steel through solid solution and precipitation hardening. Also it aids in grain refinement. Manganese improves the strength through microstructural modifications, grain refinement, solid solution and precipitation hardening. Again, nickel not only enhances solid solution hardening but also aids in precipitation of niobium carbides. Among the process parameters, slab reheating temperature (SRT) has an important role in promoting precipitation hardening during TMCP by way of retaining more precipitatable solutes within the deformed austenite. The amount of deformation, finish rolling temperature and cooling rate as a whole play significant role in grain refinement, dislocation hardening and texture hardening.

But in practice, most of the steels do not have the optimum balance in the composition and process parameters for utilisation of all the hardening effects equally. There exists one particular strengthening effect, which dominates the cause of the strength improvement due to alloying addition, and/or thermomechanical controlled processing. So clustering the steel according to its major strength contributing mechanism can help to develop a proper understanding about the system. As well it ensures efficient designing of the composition and process parameters of the steel. To develop SOM network in this direction some data values are assigned to the network, which are so chosen as to get definite biases for a particular strengthening mechanism. The plot of the values, when mapped as input vector, is found to have a well-distributed feature in the input space (Fig. 9). The SOM is trained with six neurons representing the six hardening mechanisms of steel. After sufficient learning (5,000 epochs), the neurons are found to be evenly mapped in the input space (Fig. 10). But the capacity of the network to cluster unknown data is found to be poor and has failed to follow from the metallurgical principles.

5. The Learning Vector Quantisation Model

To avoid the above-mentioned limitation of the SOM model, LVQ method is adopted to impart a certain amount of supervision in the learning process. Here also the data used are given to contain definite biases for a particular strengthening mechanism. Thus all the data have target clusters, which are the six hardening mechanisms, mentioned above. The target classes are named as:

1 for precipitation hardening
2 for grain refinement
3 for microstructures
4 for solid solution hardening
5 for dislocation hardening
6 for texture hardening

The network has 16 inputs, viz. carbon, manganese, silicon, nickel, chromium, molybdenum, copper, niobium, titanium, boron, slab reheating temperature, deformation in three different temperature zones, finish rolling temperature and cooling rate. Each input is normalised within the range of 0 to 1 by the operation given below:

\[ x_N = \frac{x - x_{\min}}{x_{\max} - x_{\min}} \]  \hspace{1cm} (1)

where \( x_N \) is the normalized value of a variable \( x \), \( x_{\max} \) and \( x_{\min} \) are the maximum and minimum values of \( x \) respectively. The input vectors are initially divided into 16 subclasses through competitive learning. Then these sixteen subclasses are linearly designated to the six target classes. Figure 11 shows the training pattern of the network having good convergence. The simulation results of the training input data with the trained network show that all the data are divided into the classes they have been designated to. The network prediction with the unknown scattered data has been quite logical and conforming to the understanding of the Physical Metallurgy principles. Some examples of the clustering with unknown normalised input data are shown in Table 1.
6. Discussion

It is known that the individual effects of niobium and titanium on the strength of the steel are increased manifold when they are added in combination with boron. So the addition of both niobium and titanium in boron treated steel has the highest improvement of strength. Thus steels can be divided into strength levels in accordance with the addition of these elements, when other composition and process parameters are kept constant. The self-organising map is found to be quite capable of clustering the steel data according to the above-mentioned elements. To optimise the number of neurons for the particular model, the prediction results of the networks with four, six and eight neurons are analysed. It is seen that the network with six neurons performs best in mapping the data, which is clustered into five groups. This is due to the fact that a four-neuron network is, by default, incapable of mapping the data in five clusters. On the other hand the six-neuron network is sufficient in respect of the number of data clusters it has map onto. Only one extra neuron remains unused in this case whereas three neurons are to remain unused in eight-neuron network. Higher the number of neurons to remain unused in a network, higher will be the chances that the unused networks randomly identify themselves with the five cluster specific neurons and thereby introduce more errors in mapping.

The input weights assigned to the three inputs by the six neurons are plotted in Fig. 8. The figure shows that the first two neurons, which map the clusters having single addition of niobium and titanium, have high assigned weights for these two elements. The next two neurons are found to have assigned the trained weights to map the data having combined addition of niobium or titanium with boron. The fifth neuron has mapped the data having all the three elements. So it is seen that the neurons after training are assigned with weights in such a way as to distinguish the data harmonious with the cluster they belong to. The sixth neuron is actually unused, as the data is clustered into five groups only and has not changed much during training.

But the process of self-organising mapping is found less effective when a huge data for all the ten composition and the six process parameters are fed to map them according to their dominant strengthening mechanism. It is required to train them with certain supervision so as to connect the neurons to its correct destination of data clusters. The network is trained with linear vector quantisation process. From the knowledge of physical metallurgy it may be stated that among the six strengthening mechanisms, precipitation hardening is caused by the elements like carbon, manganese, nickel, copper, niobium, titanium and boron; as regard to the process parameters, deformation in the non-recrystallisation and the two-phase regions as well as the finish rolling temperature have such effects. The grain refinement is mainly caused by the elements like manganese, copper, niobium and titanium and process parameters like low slab reheating temperature, high deformation in various stages and low finish rolling temperature. Carbon, manganese, silicon, molybdenum, chromium, niobium, titanium and boron along with the deformation in the non-recrystallisation region and also the cooling rate are the factors governing the microstructural manipulations while strengthening HSLA steel. On the other hand, carbon, manganese, silicon, nickel, copper, molybdenum and chromium influence the solid solution hardening. Strengthening due to dislocation hardening is achieved by high amount of deformation in the non-recrystallisation and the two-phase region and by subsequent cooling at a higher rate. Combined effects of molybdenum, nickel and titanium help to enhance it. The texture hardening is the result of high deformation in the two-phase region. Keeping the above facts in mind, the datasets of input variables are chosen in such a way that only one of the strengthening mechanisms may operate.

The neurons are trained to map these data clusters and are found to predict the dominant strengthening mechanism acting on a thermomechanically processed HSLA steel quite effectively (Table 1). Table 1 demonstrates that...
grain refinement is the dominant strengthening mechanism for alloy 1 where all the process parameters are highly favourable for achieving smaller grain size. It is known that low slab reheating and finish rolling temperatures along with high amount of deformation percentage in the three stages followed by a high cooling rate lead to considerable grain refinement in a steel, which contains high microalloying elements *viz.* niobium and titanium. Incidentally the major solid solution strengthening elements like molybdenum and chromium are absent in this alloy. The present network is therefore found to corroborate with the existing knowledge of physical metallurgy.

When an alloy does not contain niobium or titanium, but contains higher amount of molybdenum, chromium and silicon it is expected that the above alloy will experience solid solution strengthening provided that the slab reheating temperature is high enough to dissolve all the substitutional elements and the deformation in each stage is small enough to prohibit strain induced precipitation. This metallurgical belief is amply supported by the network prediction that solid solution hardening is the dominant strengthening mechanism for alloy 2. Similar arguments are applicable for the other predictions listed in Table 1. Thus it is clear that the network prediction with unknown data is compatible with the theoretical predictions, which follow from Physical Metallurgy principles.

### 7. Conclusion

1. The self-organising map is found to be quite capable of clustering the steel data according to its alloying additions.
2. The process of self-organising mapping has certain limitation to map huge data concerning all the ten compositional and six process parameters.
3. The data can be successfully mapped according to their dominant strengthening mechanism with certain degree of supervision using Learning Vector Quantisation.

### REFERENCES