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Neural Network Based Adaptation Algorithm for Online Prediction of Mechanical Properties of Steel

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ABSTRACT

After production of a steel product in a steel plant, a sample of the product is tested in a laboratory for its mechanical properties like yield strength (YS), ultimate tensile strength (UTS) and percentage elongation. This paper describes a mathematical model based method which can predict the mechanical properties without testing. A neural network based adaptation algorithm was developed to reduce the prediction error. The uniqueness of this adaptation algorithm is that the model trains itself very fast when predicted and measured data are incorporated to the model. Based on the algorithm, an ASP.Net based intranet website has also been developed for calculation of the mechanical properties. In the starting Furnace Module webpage, austenite grain size is calculated using semi-empirical equations of austenite grain size during heating of slab in a reheating furnace. In the Mill Module webpage, different conditions of static, dynamic and metadynamic recrystallization are calculated. In this module, austenite grain size is calculated from the recrystallization conditions using corresponding recrystallization and grain growth equations. The last module is a cooling module. In this module, the phase transformation equations are used to predict the grain size of ferrite phase. In this module, structure-property correlation is used to predict the final mechanical properties. In the Training Module, the neural network based adaptation algorithm trains the model and stores the weights and bias in a database for future predictions. Finally, the model was trained and validated with measured property data.

1. Introduction

Prediction of mechanical properties of hot rolled plates using principles of microstructural evolution and structure-property correlations is a challenging task for researchers. This paper describes the methodology of prediction of mechanical properties of hot rolled plates of both C-Mn and microalloyed grades of steel using a mathematical-artificial neural network (ANN) hybrid model. The basic mathematical model is developed from the theoretical equations of microstructure evolution during reheating, deformation, recrystallization, grain growth, phase transformation and structure-property correlation. The initial coefficients and exponents of the semi-empirical equations were determined from the experimental data generated through experimentation in dynamic thermo mechanical simulator and experimental rolling mill. The mechanical properties predicted by the empirical

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models are not highly accurate as the empirical equations have been formulated with some simplified assumptions which are not suitable for practical industrial application. Therefore, the mathematical model is combined with an ANN model in an innovative way to predict mechanical properties of plates more accurately. The uniqueness of this combination is that the model trains itself very fast when predicted and measured data are incorporated to the model.

An ASP. Net based website has been developed to simulate plate rolling conditions and predicts the mechanical properties in the intranet of Steel Authority of India Limited (SAIL). Through the SAIL intranet, the model system is accessible to all SAIL steel plants, marketing centres and other units throughout India. The website has 4 major web pages. In the Furnace Module webpage, the austenite grain size of the product is calculated using semi-empirical equations of austenite grain size during heating of slab in a reheating furnace. In the Mill Module webpage, different conditions of static, dynamic and metadynamic recrystallization are predicted. Austenite grain size is calculated from the recrystallization condition using corresponding recrystallization and grain growth equations. In the cooling module, the phase transformation equations are used to predict the grain size of ferrite phase. The structure-property correlation is applied in this module to predict the final mechanical properties like yield stress, ultimate tensile strength and percentage elongation. The Hybrid Module webpage uses the hybrid ANN module to predict the final properties of plates.

2. Literature Review

The objective of the literature search is to find out empirical equations developed by different researchers for prediction of mechanical properties of steel. Following pioneering works of Sellars and Whiteman [1,2] pioneered the work of development of models for predicting microstructure evolution during hot rolling in the late 1970s using empirical equations which led to direct industrial application in early 1990s. Siwecki [3] has described details microstructure-evolution model for hot rolling and its application to forecasting the microstructure evolution during recrystallization controlled rolling of Ti-V-N and Ti-V-Nb microalloyed steels. Kern et al [4] have developed computer models for the simulation of grain size development during thermo-mechanical rolling and the resulting strength properties for the prediction of the material properties of microalloyed HSLA steel plates. The standard deviation between predicted and measured properties for YS and UTS is about 30N/mm2. Saito and Shiga [5] of Kawasaki Steel Corporation have developed a computer simulation model of microstructural evolution on the basis of chemical thermodynamics and classical nucleation and growth theory. A review paper was published by Senuma et al [6] describing mathematical models for predicting microstructural evolution and mechanical properties of hot strips. The successful application of computer modeling contributes to quality improvement and cost reduction through optimum design and control. Suhirii et al [7] discussed a microstructural evolution model for high carbon (0.5% C) steels. The mathematical model predicts the transformation kinetics during cooling with special attention to pearlite transformation aiming at the application to high carbon steels. Herman et al. [8] developed an empirical model for precipitation kinetics during hot rolling HSLA steels. They have prescribed two different equations for precipitation kinetics: one for uncrystallized austenite and other for recrystallized austenite. Hodgson & Gibbs [9] developed mathematical models for each of the microstructural events that occur during the hot rolling for a wide range of commercial steels. These models have been incorporated into process models for the various mills to allow the prediction of final mechanical properties. Siciliano et al [10] developed a mathematical model which correlates Mean Flow Stress (MFS) with chemical composition, strain, strain rate and temperature. The prediction falls in the range of +/- 15%.

With development of soft computing techniques like artificial neural network (ANN), genetic algorithm (GA) etc, efforts have been made by many researchers to predict mechanical properties of hot rolled steel. Bhadeshia [11] has described the application of neural network in different fields of material science. He suggested that mechanical properties need to be expressed in quantitative model as a function of large number of process variables. Dumortier and Lehet [12] describes a statistical modelling of mechanical tensile properties of steels by using neural networks and multivariate data analysis based on the data obtained from Hot Strip Mill of Cockerill-Sambre Carlam Steel Plant. They have developed an ANN model with target variables as Yield strength [Re], Ultimate Strength [R], Elongation [EI] with input variables as thickness [Th], width [W], steel chemical analysis like [C], [Mn] and [P] and reheating temperature [TF], roughing temperature [TS], finishing temperature [TR] and coiling temperature [TC]. Datta et al [13] described an Petri Neural Network model (a multilayered feed forward network model) used for predicting mechanical properties of steel. Warde and Kimowles [14] predicted yield strength of polycrystalline superalloys using a artificial neural network within a Bayesian framework. Femminella [15] described the importance of data pre-processing and model initialization.
3. Hybrid Model Development

The on-line hybrid model has been developed in a series of steps which include selection of empirical equations, development of mathematical model, and development of Mathematical-ANN hybrid model and integration of the hybrid model with plant automation system to predict the mechanical properties on-line.

3.1 Selection of Empirical Equations

As discussed earlier, a large number of empirical relationships are published in the literature. The equations are converted into generalized form and given below (eqn. 1 to 14). The nomenclature used in the equations is given in Table-1.

The grain growth equation during reheating is given by,

\[ D_b = A.t^m . e^{-Q/RT} \]  

(1)

During deformation in the rolling process static recrystallization (SRX), dynamic recrystallization (DRX), metadynamic recrystallization (MDRX) and grain growth takes place. Empirical equations for these processes are given below:

Peak strain, \( \epsilon_p = a_c . \dot{\epsilon}.d^e_o . e^{Q/RT} \)  

(2)

Critical strain \( \epsilon_c = a_c . \dot{\epsilon}.d^e_o . e^{Q/RT} \)  

(3)

RX grain size, \( d_i = a_c . \dot{\epsilon}.d^e_o . e^{Q/RT} \)  

(4)

MDRX grain size, \( d_m = a_c . \dot{\epsilon}.d^e_o . e^{Q/RT} \)  

(5)

Table 1. Description of symbols used in formula
Time required for 50% of static recrystallization is given by,

\[ t_{0.5\alpha} = a c \cdot e^{-\frac{d_s}{0.639 r}} \]  \hspace{1cm} (6)

Volume fraction of SRX, \( X_{\alpha} = 1 - e^{-\left(\frac{t}{t_{0.5\alpha}}\right)^{0.5}} \) \hspace{1cm} (7)

where \( k = a c \cdot d_s \cdot e^{\frac{Q}{RT}} \) \hspace{1cm} (8)

SRX grain size, \( d_{\alpha} = a c \cdot d_s \cdot e^{\frac{Q}{RT}} \) \hspace{1cm} (9)

SRX grain growth \( d^n = d_\alpha^n + a(t - b_{0.5}) \cdot e^{\frac{Q}{RT}} \) \hspace{1cm} (10)

Ferrite grain size after cooling is given by

\[ d = (1 - a)^{(b + cC + (d + eC) \cdot C + f(1 - e \cdot \gamma))^0.5} ] \]  \hspace{1cm} (11)

where, \( C = [\%C] + [\%Mn]/6 \)

Experiments were conducted in Dynamic Thermo Mechanical Simulator, Gleeble 3500 to find stress, strain and ferrite grain size for at different strain rates and temperatures. Using the data generated in the Gleeble3500, the coefficients and exponents of the above equations were determined by parameter estimation technique minimizing root mean square error using a multiple multivariable optimization technique. The details of the technique are described in an earlier publication \[25\]. The initial values of the coefficients required for the optimization were taken from literature \[26\] and \[27\].

The structure-property correlation equations were also generalized as follows:

The generalized form of yield stress(YS) of material is given by

\[ \sigma_y = a + b[C] + c[Mn] + d[Si] + d[N_r]^{0.5} + ed_{\alpha}^{0.5} \]  \hspace{1cm} (12)

Similarly, ultimate tensile strength(UTS) is given by,

\[ \sigma_t = a + b[C] + c[Mn] + d[Si] + d[P] + f[N_r] + gd_{\alpha}^{0.5} \] \hspace{1cm} (13)

Percentage elongation(%El) is given by,

\[ \epsilon_r = a - b[C] + c[Mn] + d[Si] - d[P] - f[S] - gd_{\alpha}^{0.5} \] \hspace{1cm} (14)

The coefficients of the above mechanical properties equations proposed by different researchers are well documented in the books of Lenard et al \[26\] and Ginzburg \[27\]. Different researchers have proposed different equations for the three properties. The approach adopted in this present work was not to evaluate the equations proposed by individual researchers. All the equations were taken as components of the hybrid model.

### 3.2 Development of Mathematical Model

A mathematical model has been developed on the modular design approach. The plate mill line has been divided into 3 parts: reheating furnace, mill stand and cooling zone. Individual modules have been developed for prediction of grain size after each part separately and then these parts have been integrated. Based on the above concepts, computer program has been written in ASP.Net as front page and VB.Net programming language for model calculations. It calculates strain, critical strain and conditions for dynamic recrystallization. When there is a dynamic recrystallization, the model calculates dynamic recrystallization fraction. Based on recrystallization kinetics, the model predicts grain size after the pass. After calculation of austenite grain size after mill stand, the cooling module calculates phase transformation kinetics from austenite to ferrite. This calculation is made by incorporating cooling rate and composition to phase transformation equations. After the grain size of each phase and their fraction is calculated, the model calculates final mechanical properties: YS, UTS and % elongation.

### 3.3 Development of mathematical-ANN hybrid model Adaptation Algorithm

The mechanical properties predicted by the empirical models are not highly accurate as the empirical equations have been formulated with some simplified assumptions which are not suitable for practical industrial application. Therefore, an ANN program has been used along with the mathematical model as shown in Figure 1.

![Figure 1. Conceptual Diagram of Hybrid Model](https://example.com/figure1.png)

The mechanical properties predicted by the empirical models are not highly accurate as the empirical equations have been formulated with some simplified assumptions which are not suitable for practical industrial application.
Therefore, an ANN program has been used along with the mathematical model as shown in Figure 1. Each of the mechanical property has been trained with ANN model with training data. In the standalone ANN model, the inputs and the measured outputs are used for training of the model. In the present work, the empirical model output is considered as one of the inputs to ANN model. In a standalone ANN model, the output parameter is mapped to those input parameters which influence it. In this case the outputs, which are mechanical properties, are highly influenced by microstructural evolutions during rolling. The calculated grain size by empirical equation is the result of all microstructural evolution phenomena such as SRX, DRX, MDRX and Grain Growth. Therefore, the empirically calculated mechanical property is considered as one of the input parameters in this model.

Figure 1 also shows the structure of the ANN model used for the hybrid modelling. It consists of one input layer of 8 nodes, one output layer with 1 node and one hidden layer with two nodes. The ANN network is a feed forward network in which the node value at each hidden node is calculated by multiplying weight factors to input parameters and adding bias value to it. A transfer function (TF) is used for normalization of the hidden layer value. In this case the TF is chosen as a sigmoid function so that all the calculated values are normalized between 0 and 1. The training program of the ANN model is written with variable learning rate and conjugate gradient technique of error minimisation as discussed in an earlier publication (Rath et al. [28]).

3.4 Development of Intranet Simulation Website

The hybrid model is coded in ASP.NET using VB.NET programming language. The front end of the program is series of “.aspx” files with cascading style sheet (CSS). The back end of the program is equipped with Microsoft SqlServer RDBMS which is connected to the ASP.NET program using Microsoft.Net framework object SQLClient.

The simulation website has 4 major web pages: Furnace Module page, Mill Module page, Cooling Module page and Hybrid Module Page. The user can enter the rolling parameters like furnace reheating temperature, reduction schedules, speed schedules, temperature, and roll diameter in graphical user interface in the web-browser. The website output will show the predicted austenite grain size, ferrite grain size and hybrid model predicted mechanical properties.

The web-portal is hosted at a web server at Ranchi through ISS Server software and is available for use in the entire SAIL (a steel producing company of India) network throughout India.

The data flow diagram of the website is given in Figure 2. This figure shows that the ASP.Net program interacts with Mathematical model, ANN model and hybrid model to predict the mechanical properties. The data of the program is stored in a MS-SQL database. The model is broadcasted to SAIL.Net through Microsoft Internet Information Services (ISS) server. Users in any location of SAIL office in the country can access the program and simulate the plate rolling condition and calculate the mechanical properties.

4. Results and Discussion

The model has been validated with data obtained from New Plate Mill, Rourkela Steel Plant. Process parameters and measured properties data of 290 plates of C-Mn grade of steel and 37 plates of Microalloyed grades rolled in the mill were used for validation of the model. A validation plot for is shown in Figure 3. This plot shows that there is close match between predicted and measured YS.

Figure 4 shows the histogram of Model Error. The Model error is slightly skewed towards right. It also shows that the model predicts exactly same value as measured value for 20% cases indicating the accuracy of the hybrid model is very high.

**Figure 3. Validation of YS for Micro-alloyed Steel**

Figure 4 shows the histogram of Model Error. The Model error is slightly skewed towards right. It also shows that the model predicts exactly same value as measured value for 20% cases indicating the accuracy of the hybrid model is very high.
The summary of ranges of model prediction error is given in Table-2. This table shows that the model prediction is highly accurate for prediction of mechanical properties of Plain Carbon and Microalloyed grades of steel. However, the prediction error for elongation prediction is higher. It was found that the measured that are given in the form of integer value and decimal points are neglected which is responsible for this error.

Table 2. Model prediction Error Ranges

| Grade       | Property | Error Range (%) |
|-------------|----------|-----------------|
| Plain Carbon| YS (MPa) | -5 to +5        |
|             | UTS (MPa)| -4 to +4        |
|             | Elongation| -10 to +10      |
| Microalloyed| YS (MPa) | -8.0 to +8.0    |
|             | UTS (MPa)| -5.0 to +5.0    |
|             | Elongation| -10 to +9.0     |

5. Conclusion

A mathematical-Artificial Neural Network (ANN) based hybrid model has been developed under this work to predict the mechanical properties of hot rolled plates. The model has been validated with plant data and found to be accurate in prediction. An intranet website has been developed for simulation of process conditions and prediction of mechanical properties.

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