The 8th International Conference on
Computer Science & Education (ICCSE 2013)
April 26-28, 2013. Colombo, Sri Lanka

Prediction of the Mechanical Properties of Hot-rolled C-Mn Steels by Single Index Model

Yang Weng, Yonghong Zhao
College of Mathematics
Sichuan University
Chengdu, China, 610064

Guangbo Tang, Zhengdong Liu
Institute for Structural Materials
Central Iron and Steel Research Institute
Beijing, China, 100081

***Abstract*—semi-parametric single index model based approach is proposed for prediction of mechanical properties of hot rolled strip in this paper. Based on industrial production data, a semi-parametric single index model is developed by choosing the appropriate kernel function and window width to predict the yield strength, tensile strength and elongation. When data samples are limited, compared with regression method and neural network method, the prediction results show that the semi-parametric single-index model based method is more adaptive and the prediction performance is superior to both regression and neural network methods.**

***Index Terms*—hot strip rolling, mechanical property prediction, regression analysis, neural network, semi-parametric single-index model.**

I. Introduction

As a promising and useful technology, the mechanical property prediction for hot rolled strip can be applied to reducing the amount of sampling, controlling strip mechanical properties, in the design of new steel grades and new processes, as well as maintaining high process stability and production quality and other aspects [1], [2]. Therefore the issue of mechanical properties prediction for hot rolled strip has received extensive attentions in recent years worldwide.

Recently, a number of mechanical properties prediction models for hot rolled strips were proposed to accurately predict and control the quality of hot-rolled products. These models were developed based on the chemical composition of strips and production processes, including reheating, rolling and cooling process. According to the different modeling methods, the mechanical property prediction model for hot rolled strip can be divided into two categories, namely the metallurgical mechanism model and the statistical model [3], [4],[5].

Metallurgical mechanism models can reveal microstructure evolution of the hot rolled strip to predict its mechanical properties during the rolling process[3], [4]. Although the metallurgical mechanism models can be used for a wide range of rolling processes, the structure of these models are very complex and quite a lot of dependencies, e.g. size and volume fraction of precipitates, size and volume fraction of every transformed phases, etc., are difficult to obtain during the hot rolling process, which limits the prediction accuracy of these models. On the other hand, statistical models are developed by real production data from specific production line. These models are usually more accurate than metallurgical mechanism models, while the adaptability of statistical models are limited and they can be only used for the hot rolling process on specific production line where the data are collected from [5]. In the statistical models for hot rolled strip mechanical properties prediction, the most popular way is multivariate regression analysis. The regression analysis based approach can describe the correlations between chemical compositions of strips, processing parameters (e.g. reheating temperature, start and finish rolling temperature, coiling temperature, rolling force, etc.) and mechanical properties of hot rolled strips.

In this paper, a semi-parametric single index model based approach is proposed for mechanical properties prediction of hot rolled strips. Single index model can describe complex non-linear correlations between dependent and independent variables. Moreover, this semi-parametric method is more flexible, robust and more attractive for avoiding "curse of dimensionality" in high dimension data analysis problem [6]. The prediction results show that the semi-parametric single index model based approach is more accurate than both regression method and neural network method with limited training data.

II. Semi-parametric single index Model

In statistics, regression analysis includes any techniques for modeling and analyzing several variables, when the focus is on the relationship between a dependent variable and one or more independent variables. More specifically, regression analysis estimates the conditional expectation of the dependent variable given the independent variables, which is to estimate the relationship between the independent variable and the dependent variables $X = (X_1, X_2, \cdots, X_p)^T$ via $m(x) = E(Y|X = x)$, where $x = (x_1, x_2, \cdots, x_p)^T$, $m(x) = m(x_1, x_2, \cdots, x_p)$. In the multiple linear regression models, it is assumed that the conditional mean relationship between the response and each of the predictors is linear, i.e. that $m(x)$ is of a linear form. The most flexible models do not make any assumption about the form of the p-variate function . The problem then is to fit a p-dimensional surface to the observed data $\{(X_i^T, Y_i, i = 1, 2, \cdots, n\}$. An obvious approach is to try to generalize the univariate smoothing techniques, there is a serious problem arising: the so-called "curse of dimensionality" [7]. A popular way to overcome the dimensionality problem is to first project

978-1-4673-4463-0/13/$31.00 ©2013 IEEE

all covariates $X = (X_1, X_2, \cdots, X_p)^T$ onto a linear space spanned by the covariates and then to fit a nonparametric curve to their linear combinations. This leads to the single index model $E(Y|X = x) = G(\theta^T x)$, that is

$$Y = G(\theta^T x) + \varepsilon, \quad (1)$$

where ε is an independent random variable with zero mean and bounded variance. The task is now to estimate the unknown univariate link function $G(\cdot)$ and the p-dimensional projection parameter θ .

A. *Estimation of the Parameters and Link Function*

The parameters and the link function in the single-index model can be estimated by the following three steps.

1. : For a given value θ, the regression function $G(z|\theta) = E(Y|\theta^T X =)$ can be estimated using any nonparametric univariated smoother, such as a local weight average estimator. Due to a datum point remote from z carries little information about the value of $G(z)$, let $K(\cdot)$ be a real valued function assigning weights. The function $K(\cdot)$ is called kernel function (typically a symmetric probability density function). Let h is a bandwidth, which is a nonnegative number controlling the size of local neighborhood. Denote $K_h(\cdot) = h^{-1}K(\cdot/h)$. If a suitable kernel function $K(\cdot)$ and bandwidths h can be chosen, then is particularly easy to estimate by Nadaraya-Watson kernel estimator
$$\hat{G}(z) = \sum_{i=1}^{n} K_h(Z_i - z)Y_i / \sum_{k=1}^{n} K_h(Z_i - z) \quad (2)$$
where $Z_i = \theta^T X_i, z = \theta^T X$.
From a function approximation point of view, the kernel estimator uses local constant approximation which is unsatisfactory, and a local polynomial fit is desirable [9]. This method has a large order of bias when estimating a curve at a boundary region. Indeed, it is shown that the local linear fit is efficient in correcting boundary bias. Assume that has a continuous second derivative. For Z in a small neighborhood of z, $G(\cdot)$ can be approximated locally by a linear function, i.e.
$$G(Z_i) \approx G(z) + G'(z)(Z_i - z)$$
denote $G(z) = a, G(z_j) = a_j$, $G'(z) = a, G'(z_j) = a_j$ and $X_{ij} = X_i - X_j$The solution vector is provided by weighted least squares theory and is given by
$$\begin{pmatrix} a_j \\ d_j \end{pmatrix} = \left\{ \sum_{i=1}^{n} K_h(\theta^T X_{ij}) \begin{pmatrix} 1 \\ \theta^T X_{ij}/h \end{pmatrix} \right.$$
$$\left. \begin{pmatrix} 1 \\ \theta^T X_{ij}/h \end{pmatrix}^T \right\}^{-1} \cdot \sum_{i=1}^{n} K_h(\theta^T X_{ij}) \begin{pmatrix} 1 \\ \theta^T X_{ij}/h \end{pmatrix} Y_i]$$
2. We may estimate θ by selecting that orientation θ which minimizes
$$Q(\theta) = \sum_{j=1}^{n}\sum_{i=1}^{n} (Y_i - a_j - d_j\theta^T X_{ij})^2 K_h(\theta^T X_{ij}), \quad (3)$$
that is ,
$$\theta = \left\{ \sum_{i,j} K_h(\theta^T X_{ij})(d_j)^2 X_{ij} X_{ij}^T \right\}^{-1} \cdot \sum_{i,j} K_h(\theta^T X_{ij}) d_j X_{ij}(y_i - a_j) \quad (4)$$
3. Set θ to be the estimate obtained in Step 2 and repeat Steps 1 and 2 until prescribed convergence criteria are met. This estimator has very good asymptotic properties. It needs no under-smoothing for the estimator of θ to achieve the root-n consistency.

A natural question is how wide the local neighborhood should be so that the local approximation is valid. This is equivalent to asking how large the bandwidth parameter h should be in (2) or (3). If we take a very small , the modeling bias will be small. However, since the number of data points falling in this local neighborhood is also small, the variance of the estimated local parameters will be large. On the other hand, a too large bandwidth can cause a large modeling bias.

B. *Kernel Function Selection*

In nonparametric functional estimation, the kernel function assigns different weights to each datum point. The weights depend on the bandwidth and the estimator that are used. The function $K(\cdot)$ is usually a symmetric probability density function satisfying the following conditions,

$$K(z) \geq 0, \int K(z)dz = 1, \int zK(z)dz = 0. \quad (5)$$

Commonly used kernel functions include the Gaussian kernel, and the "symmetric Beta family", the tricube kernel function, the Epanechnikov kernel function etc. In this paper, the Gaussian kernel is chosen

C. *Bandwidth Selection*

The choice of the bandwidth parameter is rather crucial and this should be done with a lot of care. Various existing bandwidth selection techniques can be adapted for the above estimation. When is the Gaussian kernel function, the ideal optimum choice of bandwidth is the one that minimizes the asymptotic Mean Integrated Squared Error (MISE) [8], resulting in,

$$\hat{h} = 1.06\hat{\sigma}n^{-1/5}, \quad (6)$$

where $\hat{\sigma}^2$ is conditional variance estimator of Y given $X = x$. However, this asymptotically optimal bandwidth depends on unknown quantities, and hence is not directly applicable in practice. Commonly used other methods for bandwidth selection in nonparametric estimation are cross-validation techniques, plug-in methods and nearest neighbor bandwidths. In this paper, we apply leave-one-out cross-validation, that is, the bandwidth parameter is selected by minimizing,

$$CV(h) = \sum_{j=1}^{n} (Y_i - \hat{G}^{-i}(Z_i, \theta))^2, \quad (7)$$

where $\hat{G}^{-i}(\cdot)$ is the estimator without using the i-th observation. Its leave-one-out estimator is given by

$$\hat{G}^{-i}(z) = \frac{\sum_{j \neq i} K_h(Z_j - z)Y_j}{\sum_{k \neq i} K_h(Z_k - z)} \quad (8)$$

III. Results and Discussions

A. Data processing

In this paper, we mainly discuss the case of limited training data for mechanical properties prediction of hot rolled strips. Therefore, 60 data of C-Mn steel strips are selected to establish the prediction model, including chemical compositions, processing parameters and mechanical properties. In general, the impact factors of microstructure evolution and mechanical properties of hot rolled strips include chemical compositions of strips and processing parameters during the rolling process. For C-Mn steel, the chemical compositions that should be considered include: the mass fraction of elements C, Si, P, N, Mn, Al; the processing parameters that should be considered include: strip thickness, reheating temperature, reheating time, start and finish rolling temperature, cooling rate, coiling temperature, etc.

For the selected C-Mn steel production data in this paper, the element content of Al and S are stable. Therefore, the mass fraction of elements C, Si, P, N and Mn are selected as chemical composition parameters in the prediction model. Among hot rolling processing parameters, the slab have uniform thickness, the difference between rough rolling entry temperature and reheating temperature as well as the difference between rough rolling exit temperature and finish rolling entry temperature follow certain rules, in which part of the parameters have linear correlation such like reheating temperature and rough rolling entry temperature, cooling time and temperature difference between finish rolling exit temperature and coiling temperature, etc. Therefore, the selected processing parameters in prediction model include rough rolling entry temperature θ_1, finish rolling entry temperature θ_2, finish rolling exit temperature θ_3, coiling temperature θ_4, strip thickness d and cooling time t. The mechanical properties that should be predicted include yield strength σ_s, tensile strength σ_b and elongation δ.

B. The results of linear regression model

The selected chemical compositions and processing parameters of hot rolled strips are modeled as dependent variables while the mechanical properties (yield strength, tensile strength and elongation) are modeled as independent variables. By stepwise regression, the empirical regression equations can be given as follows,

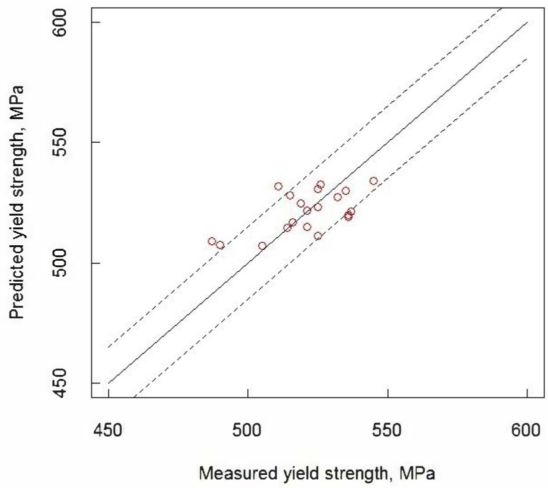

Figure 1. predicted yield strength for hot rolled strip by linear regression model.

$$\begin{aligned} \hat{\sigma}_s &= 732.8 + 140.7C + 40.4Si + 291.0P - 4.792Mn \\ &- 0.277\theta_2 + 0.067\theta_4 - 1.298t \quad (9) \\ \hat{\sigma}_b &= 524.9 + 22.9C - 50.8Si + 1650.3P + 15.4Mn \\ &- 0.211\theta_1 + 0.066\theta_3 - 1.255t \quad (10) \\ \hat{\delta} &= 20.3 + 12.5C + 6.17Si + 5.1P + 3.1Mn \\ &- 0.038\theta_2 - 0.025\theta_3 + 1.05d - 0.258t \quad (11) \end{aligned}$$

The comparison of measured and predicted mechanical properties of hot rolling strip by linear regression model for the test data set are shown in Figure 1, 2 and 3. For the yield strength and tensile strength, the prediction errors of about 80% data are less than 15MPa. The dash lines denote 15MPa interval, which are the same meaning in the following figures. For the tensile strength, the prediction errors of about 85% data are less than 12MPa. The dash lines denote 12MPa interval, which are the same meaning in the following figures. For elongation, the prediction errors of about 75% data are less than 3%. The dash line denote 3% interval, which is the same meaning in the following figures.

C. The results of single index model

In order to enable a direct comparison with the linear model, we use the same variables that introduced in linear regression model to fit the single-index model. We standardized the regressors for identifiable cases, each variable is centered by its sample mean and divided by its standard deviation, that is $x^* = (x - \bar{x})/\hat{\sigma}$ where $\bar{x}$ denotes the sample mean of x, $\hat{\sigma}$ denotes the standard deviation.

Choose an initial value of θ, which can be selected by the parametric linear model. Using the Gaussian weights and taking h to be an estimate of the bandwidth that is optimal by leave-one-out cross-validation. We applied the iterate procedure to the single-index model to obtain the fitted value.

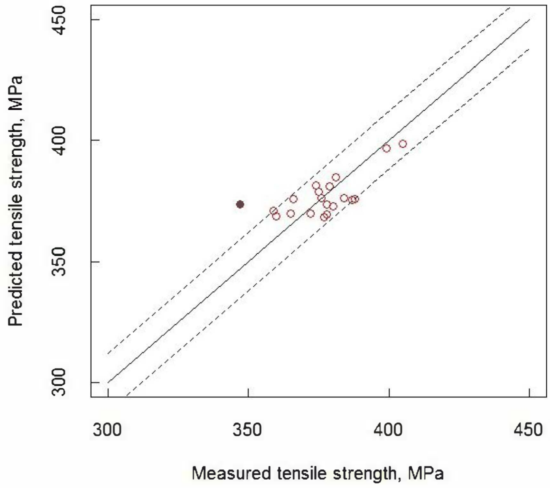

Figure 2. predicted tensile strength for hot rolled strip by linear regression model.

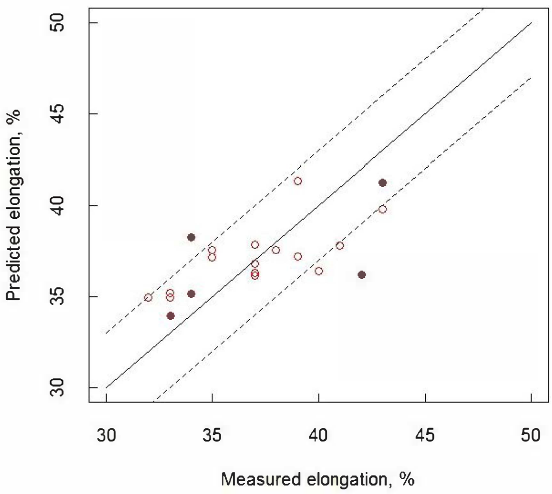

Figure 3. predicted elongation for hot rolled strip by linear regression model.

The estimated index for yield strength, tensile strength and elongation are show in Figure 4, 5 and 6, respectively.

The comparison of measured and predicted mechanical properties of hot rolling strip by semi-parametric single-index model for the test data set are shown in Figure 7, 8 and 9. For the yield strength and tensile strength, the prediction errors of about 95% data are less than 15 MPa. For the tensile strength, the prediction errors of about 95% data are less than 12MPa. For elongation, the prediction errors of more than 95% data are less than 3%. The prediction performances for all mechanical properties are significantly improved.

Table I shows the prediction performance of linear and single-index model of the test data. Compared with the linear model, single-index model have higher prediction accuracy in fitting a nonlinear relationship between covariates and response variables which leads to better prediction performance.

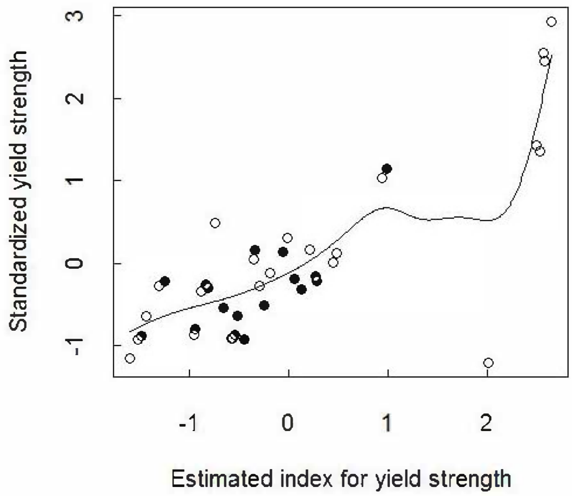

Figure 4. estimated index for yield strength.

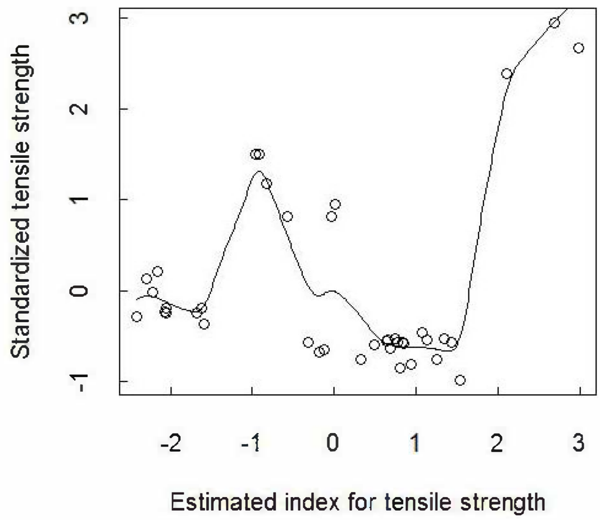

Figure 5. estimated index for tensil strength.

Table I
COMPARISON OF PREDICTION PERFORMANCE FOR MECHANICAL PROPERTIES OF HOT ROLLED STRIP

	σ_s	σ_b	δ
Linear model	10.45	9.31	2.55
Single index model	7.20	7.13	1.39

Note: The error criterion is rooted mean square error (RMSE)

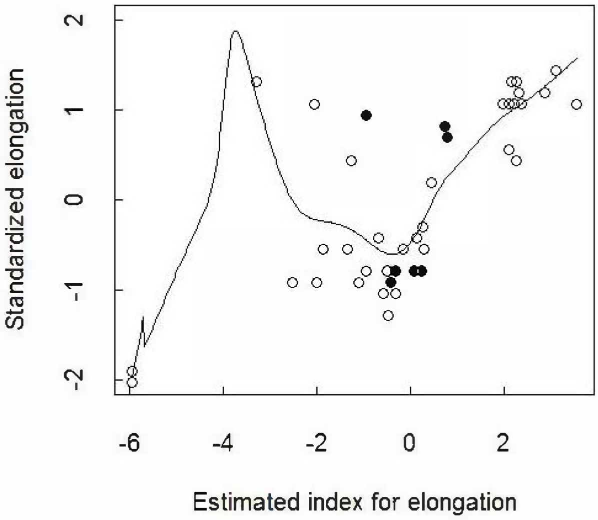

Figure 6. estimated index for elongation.

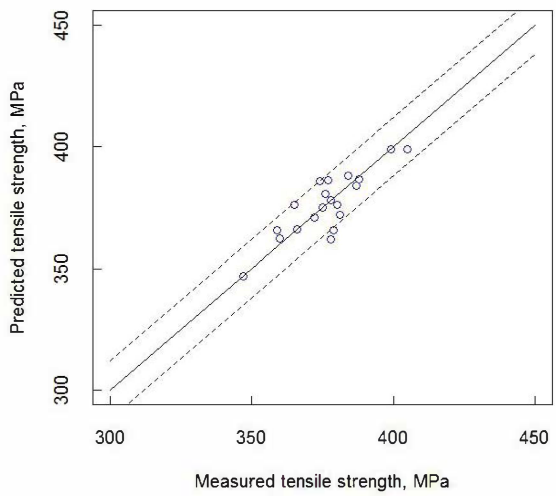

Figure 8. predicted tensile strength for hot rolled strip by single index model.

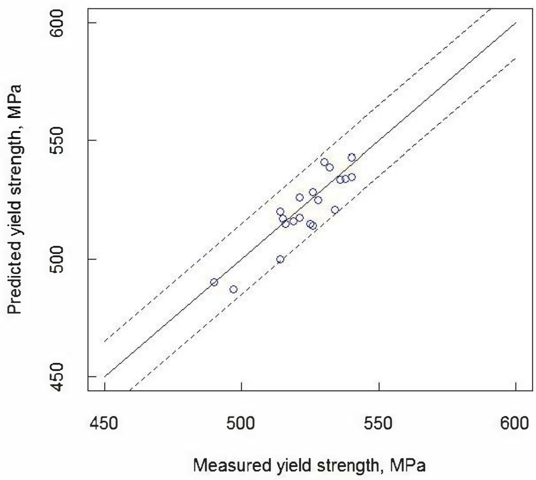

Figure 7. predicted yield strength for hot rolled strip by single index model.

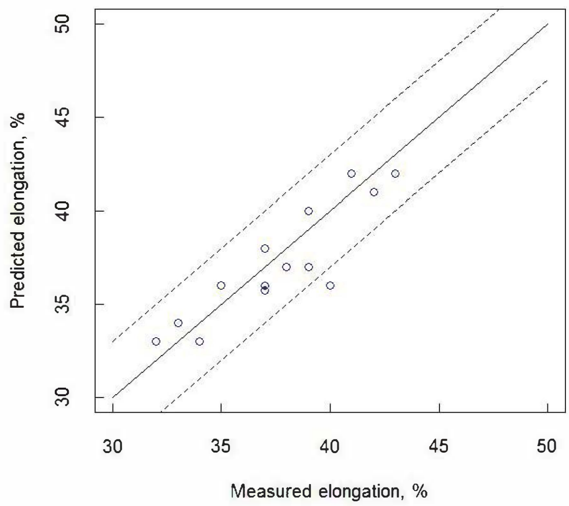

Figure 9. predicted elongation for hot rolled strip by linear single index model.

IV. CONCLUSION

In this paper, the mechanical properties prediction problem for hot rolled strip with limited training data has been discussed. The prediction models have been developed by using linear regression method and semi-parametric single index model method respectively. Compared with regression methods, the mechanical properties prediction performance of hot rolled strip can be significantly improved by using the proposed semi-parametric single-index model approach. In the case of limited training data from specific production line, the proposed method can avoid the unstable estimation on the boundary of semi-parametric model, which makes this method can be better adapted for mechanical properties prediction of hot rolled strip.

ACKNOWLEDGMENT

This work was partly supported by the National Natural Science Foundation of China (No. 61203219) and the Project of Scientific and Technical Supporting Programs of China During the 11th Five-year Plan (Nos. 2006BAE03A08 and 2006BAE03A09)

REFERENCES

[1] Gan Y, Liu Z D, Wang G D, Wu D, Wang W, Zhang P J, *On-line Application of Structure and Property Prediction System on Hot Rolling Line on 2050 HSM at Baosteel* Iron and Steel, 2006, 41(3): 39-44.
[2] Liu Z D, Dong H, Gan Y, *Application of Process Modeling to Hot Strip Rolling*, Iron and Steel, 2003; 38(2): 69-91.
[3] Sellars C M, Whiteman J A, *Recrystallization and grain growth in hot rolling*, Metal Science, 1979, 3(4): 187-194.
[4] Majta J, Kuziak R, *Use of the computer simulation to predict mechanical properties of C-Mn steel, after thermo-mechanical processing*, Journal of Materials Processing Technology, 1996, 60: 581-588.

[5] Guo Z H, Zhang Q L, Su Y C, Xia Y, *Thoughts on Mechanical Property Prediction of Hot Rolled Strip*, Metallurgical Industry Automation, 2009, 33(2): 1-6.
[6] Hardle W, Hall P, Ichimura, H, *Optimal smoothing in single-index models*, Ann Statist,1993, 21(1): 157.
[7] Kong E F, Xia Y C, *Variable selection for the single-index model*, Biometrika, 2007, 94 (1): 217-229.
[8] Silverman B W, *Density Estimation for Statistics and Data Analysis*, London: Chapman and Hall Ltd, 1986..
[9] Fan J Q, Gijbels I, *Local Polynomial Modelling and Its Applications*, London: Chapman and Hall Ltd, 1996.