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NEURAL NETWORK MODELLING FOR PREDICTION OF FERRITE NUMBER IN STAINLESS STEEL WELDS

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Abstract:- *As Neural Network (NN) has been very useful tool for recognizing a pattern in complex data, here the complex data means the complex Non-Linear inter-relationships and inter dependence among the various materials/ process parameters of the weld deposits concerned.*
There is a significant role of the ferrite content in determining the fabrication and service performance of welded structures. Because several properties can be predicted by estimating ferrite content. Research has also discovered that a minimum ferrite content in steel is very necessary to improve the hot cracking resistance whereas higher ferrite leads to higher mechanical and corrosion resistance of the ferritic-austenitic types, especially the "duplex" and "Super-duplex "types.
Though it has become the routine practice to predict the ferrite content from the schaffeler, Delong or WRC-1992 diagram. All is designed on the basis on Ni-equivalents and Cr-equivalents .But different diagrams considers different respective equivalent of Ni and Cr. But the limitations of using these diagrams lie in their linear or "pseudo-linear" relations and also they don't take in to consideration every chemical compound and the interaction between them. The relation between the variables (dependent and independent) are more complex, i.e. Non-linear behavior. this problems can be overcome by using a Neural Network modeling.we attempted Network architectures like Multilayer perceptron method, (MLP) ,and Radial basis function (RBF), for building a neural networks and algorithms like Back propogation, (BP), conjugate gradient decent (CG), quick propagation (QP),Levenberg Marquardt (LM), Delta bar delta (DD) and such many for training the NN model . By applying Neural Network Modeling, we have trained several best optimized models for prediction of ferrite Number (output) as a function of Chemical Composition (input) and Mechanical properties (Charpy toughness, Yield strength, % elongation and Ultimate tensile strength) as a function of Chemical composition and ferrite number. Neural Network models predicted the output well tuned with the experimental data and have also shown the Metallurgical trends. Successfully trained NN model has been very useful tool for the cost reduction in the welding research and practice engineering field in the terms of material, money and time saving aspects

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Key Words: *Ferrite Number, Neural Network, Austenitic Stainless Steels, Duplex Stainless Steels, Ferrite content, Alloy composition, constitution Diagram*

INTRODUCTION

1.1 Austenitic stainless steels

Very popular in the fabrication industry, as they can withstand a variety of corrosion media.

The chromium content of these steels range from 16% to 30%, and the nickel content from 5% to 35%. These are called austenitic steels, as the micro-structure of these grades is predominantly austenite. Nonetheless, there is some ferrite in several grades; the other grades which do not contain any ferrite are called fully austenitic grades. A small amount of ferrite is necessary to stop cracking during solidification of welds. However, in certain media, ferrite causes corrosion, and the only choice for such media is to opt for fully austenitic grades. Fully austenitic grades give rise to micro-fissuring during welding, which could be eliminated by choosing low heat input processes along with restricted low melting constituents in the weld metal.

1.2 Welding of Standard Austenitic SS

Weld metal of the same composition contains 4 to 12% (5 to 15 FN) delta ferrite, thus being resistant to hot-cracking, In the case of special requirements, such as welded joints required to be non-magnetic, highly corrosion resistant or tough at subzero temperatures, a fully austenitic weld metal should be chosen, because Delta ferrite is a magnetic phase Ref. Table 1.

Admixture from the base metal should be below 40% and if possible nitrogen pick-up during welding should be kept low, in order to not lower the delta ferrite too much.
In general, the 300 Series stainless steels: those which contain ferrite and austenite; and those which contain only austenite, none of the types requires any preheat or interpass temperature or post weld heat treatment. However, heating up to 150 ºC before welding is advisable to evaporate any condensed moisture in the joint
Cr-Ni austenitic type may also be joined by using Cr-Ni-Mo-consumables, but with regard to corrosion resistance, weld metal of the same composition should be preferred.

1.3 Role of ferrite

Most of austenitic-type stainless steel weldments (AWS-3XX type) show a limited
delta-ferrite content.This results from the well established relationship between a reduced sensitivity to hot-cracking and the presence of a certain amount of ferrite in the deposited metal. Higher ferrite level lead s to the higher mechanical and corrosion resistance of the ferritic-austenitic types, especially the "duplex" and "super-duplex" types.(11)

Table 1. Ferrite Specifications in Weld Metal. Source (11)

To specify a FN, we have to balance hot-cracking sensitivity and the application requirements. Here are some general guidelines, which must be adapted to the actual applications:

Non magnetic properties are required	≤0.1 FN
Specific corrosion; some heat resisting weld metals;service below-105^0 C	≤0.5 FN
General use, unstabilised weld metal from -105 ºC to + 350^{0}C	4 to 12 FN
General use, stabilized weld metal from, from -105 ºC to + 350^{0}C	6 to 15 FN
Service temperature in the stigmatization range (540 – 900 ºC)	3 to 8 FN
Ferritic-austenitic, “ duplex” and “super-duplex” type	30 to 70 FN

Table 2. Factors affecting the delta-ferrite in austenitic stainless steel weld

The weld metal composition	welding parameters	Heat treatments	The resultant mechanical and metallurgical properties
C, Si, Cr, Ni, Mo, Mn, S,P etc..	Heat input, Applied current AC or DC nature, voltage Electrode polarity, interpass temperature, Type of welding process. Etc	Pre-weld heat treatment , Post-weld Heat treatment.	Charpy impact value UTS, % Yield strength, %Elongation, % Red. Area. % Ferrite Number-FN

The sole aim of this paper is to explain the usefulness of the Neural network modeling technique as a optimum tool for recognizing the pattern among many complex weld deposits variables & to establish some relationship between input & output variables. During the last decades, many NN models in material science have been designed & developed using various Neural Networks methods . Here I have attempted Neural Network architectures like Multilayer perceptron method, (MLP) , & Radial basis function RBF, for building a neural networks & algorithms like Back propogation, (BP), conjugate gradient decent (CG), quick propogation (QP) , Levenberg Marquardt (LM), Delta bar delta (DD) & such many for training the NN model .

1.4 Some terms defined for the welding of Austenitic stainless steel are given below:

Delta-ferrite

Iron-base alloys crystallize to ferrite or austenite. Ferrite is distinguished between that which forms from the melt, Delta Ferrite, and that which forms from solid state transformation product, Alpha Ferrite.

Ferrite Number vs. Ferrite Percent:

A comparison of point counting and magnetic measurements revealedthat the ratio of ferrite number to ferrite percent was not uniform over the entire FNscale. It was established that the correlation was roughly 1:1 for FN values of O-28.However, above 28 FN the correlation deviated. Examinations, during experimentaltrials, suggested that this correlation could be approximated using a ferrite number toferrite percent ratio of 1.4:1. However, a lack of agreement between laboratories left this issue in dispute among researchers. [23][11]

Ferrite number (FN)

According to ISO 8249 - 1985 : "At present, experimental methods are not available that give an absolute measurement of the amount of ferrite in a weld metal, either destructively or non-destructively".That is why this standard and its equivalent AWS A 4.2-91 only state ferrite in terms of FN, a standardized arbitrary value, measured by calibrated magnetic instruments [11][22]

FN measurement conditions

The FN values, determined according to the two standards on as deposited all-weld metal, without any thermal influence or treatment.[22]

Prediction or estimation of ferrite content

The ferrite content of weld deposits can be estimated by means of constitution diagrams such as- Schaeffler, and DeLong diagrams. The most recently developed and more accurate WRC - 1992 – diagram extended to 100 FN, i.e. covers the duplex range.[11][21]

Ferrite number measurement

Ferrite is ferromagnetic while austenite is not. The relationship between the tear-off force, needed to pull the sample from a well-defined magnet and FN is obtained using primary standards consisting of a non-magnetic coating of specified thickness on a magnetic base.

These primary standards are only suitable for use with a few laboratory instruments such as the Magna-Gage. Secondary weld metal standards are needed to calibrate the measuring instruments usable under shop and field conditions [23]

2.0 Modeling work

In the present work, Multilayer perceptron (MLP) architectural best trained NN model has been used to estimate the ferrite content of the “duplex” & “Super-duplex” stainless steel.

This NN Mode for ferrite content prediction has been prepared with the data base consists of 248 data set, comprising composition & ferrite content of Gas metal arc welding (GMAW). Out of 248 data set partially collected from both standard welding literatures & well reputed welding industry. Out of 248 data set, only 232 data set has been used for the analysis. The NN software automatically divide 115 for training, 58 for selection i.e. validation & remainder 58 for Test as an auto sampling of case subsets.

While the remainder 16 data set (248-232) has been kept as “Un-seen”. Means, not used in the training the network. This data set has been used to check the correlation between the observed & predicted values. The correlation between observed & predicted values has been achieved 0.98 With the best trained model with Multilayer perceptron (MLP) architecture as shown result summary -table 4 & their respective graph as shown in fig.1. This practice is particularly helpful in checking whether had any “over-learning” occurred in the course of training, otherwise the given prediction may stand “vague’ or “irrelevant”. It happened whenever the model had been tried out with Radial Basis Function (RBF) & generalized regression Neural network (GRNN) architectures. Hence, the most satisfactory performance of the model is observed with a model trained by MLP technique.

The data set consists of 304, 304L, 308, 308L, 309, 309L & 316, 316L i.e 300 series Austenitic type.

Creating & Designing a Neural Network is very crucial part of the NN analysis because the performance of the model for the intended application is greatly depend on it.

Having selected the independent variable as input (composition:C,Si,Mn,Ni,Cr, Mo, N & Nb) & depended/ continuous variable FN as output. The network is to be created using different architectures the summary of different network architectures & training algorithms as shown in Table 3

Table 3 Summary of Network Architectures & Training algorithms (1)(6)(7)

Network architectures		Neural Network training algorithms	
MLP	Multilayer perceptron Network	BP	Back propagation
		CG	Conjugate Gradient Descent
		QN	Quasi-Newton
		LM	Levenberg-Marquardt
		QP	Quick Propagation
		DD	Delta-Bar-Delta
RBF	Radial Basis function Network	SS	(sub) Sample
		KN	K-Nearest Neighbor(deviation assignment)
		KM	K-Means (Center Assignment)
GRNN	Generalized Neural Network	GR	Generalized regression Neural Network training
		KM	K-Means (Center Assignment)
		KO	Kohonen(center assignment)

Network design (once the input & output variables have been selected) follows a number of stages:

Selection of initial configuration (typically, one hidden layer with the number of hidden units set to half the sum of the number of input and output units;

Iteratively conduct a number of experiments with each configuration, retaining the best network (in terms of selection error) found.

A number of experiments are required with each configuration to avoid being fooled if training locates a local minimum, and it is also best to resample.

On each experiment, if under-learning occurs (the network doesn't achieve an acceptable performance level) try adding more neurons to the hidden layer(s). If this doesn't help, try adding an extra hidden layer.

If over-learning occurs (selection error starts to rise) try removing hidden units (and possibly layers).

Neural network training algorithms are iterative, training over a period of time, and need to be repeated a number of times until a satisfactory solution is found.

The NN model for prediction of ferrite content has been best optimized using the Multi layer perceptron architecture in two phases with Back propagation algorithms i.e BP & Levenberg Marquardt i.e LM with the Network design / Configuration of 9 inputs Units (Chemical compositions) 7 Hidden Units in single layer & 01 Output (i.e FN)

The below table 4 show the concern Model Summary report with Training & Selection error as 0.011343 & 0.088 respectively.

Table 4. Model summary report for the best optimized model for prediction of FN number as a function of chemical composition.

Model Summary Report										
Profile	Train Perf.	Select Perf.	Test Perf.	Train Error	Select Error	Test Error	Training/Members	Input	Hidden (1)	Hidden (2)
MLP 9:9-7-1:1	0.052031	0.3329	0.115716	0.011343	0.88298	0.032663	BP100,LM439b	9	7	0

3.0 Result & Discussion

3.1 Prediction of the ferrite number

The ability to perform well on new data is called generalization, and is the most desirable property of a neural network. How then can we ensure that a network will generalize well? An important technique is to hold back some of the data, and not to use it for training the network. The below mentioned is the data sheet (Table 5) not used in the training. Source (1) (6) (7)

Table 5 Unseen data base (Duplex steel composition)

Carbon	Silicon	Manganese	Nickel	Chromium	Molybdenum	Copper	Nitrogen	Niobium
0.03	0.35	0.85	8.7	23	3	0	0	0
0.03	0.35	0.85	8.7	23	3	0	0	0
0.03	0.35	0.85	8.7	23	3	0	0	0
0.022	0.8	1	7.5	21.3	2.75	1.7	0	0
0.022	0.8	1	7.5	21.3	2.75	1.7	0	0
0.022	0.8	1	7.5	21.3	2.75	1.7	0	0
0.022	0.8	1	7.5	21.3	2.75	1.7	0	0
0.022	0.9	1	9	25	3.7	0	0	0
0.022	0.9	1	9	25	3.7	0	0	0
0.022	0.9	1	9	25	3.7	0	0	0
0.02	0.9	1	9	25	3.7	1	0.2	0
0.02	0.9	1	9	25	3.7	1	0.2	0
0.02	0.9	1	9	25	3.7	1	0.2	0
0.035	0.7	1.35	9	25	4	0.7	0.22	0
0.035	0.7	1.35	9	25	4	0.7	0.22	0
0.035	0.7	1.35	9	25	4	0.7	0.22	0

Testing unseen data with best network model / Making Predictions Using the Neural Networks
Since neural networks take a considerable amount of time to train, it is normal practice to keep copies of successful networks rather than recreating them each time the data is analyzed (which is the procedure often used for conventional statistical methods).Predictions can be made based on cases in the data set or new cases entered by the user. Hence the above unseen data containing composition for Duplex stainless steels has been tested to make prediction as shown in table 6.

Table 6 Prediction for given Input data (Composition of Duplex Stainless steels)

Line Number	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
Prediction	40.06	40.06	40.06	50.00	50.00	50.00	50.00	50.00	50.04	50.04	50.04	49.99	49.99	49.99	49.96	49.96

As can be seen from the above result that MLP trained models give very appropriate prediction for the ferrite content for the given "Duplex Stainless steel "composition.

3.2 Effect of alloying elements on Ferrite Number.

In WRC-1992 diagram, as Cr equivalents Cr, Mo, & Nb considered whereas it is well known that Silicon has strong influence on the ferrite content that can also be understood from this NN analysis. [Fig. 9].

The effect of silicon on weld metal ferrite had been examined by D. J. Kotecki.[13] The results of his study revealed that the 1.5 silicon weighting factor used in both the Schaeffler and DeLong diagrams was inaccurate. Kotecki's work suggested that the weighting factor be reduced to O.12012]Kotecki conducted a similar study to investigate the effect of molybdenum and concluded that its coefficient be reduced
from 1.0 to 0.7.[13]

The role of silicon in influencing FN in Stainless steel welds is clearly exhibited in Schaffer diagram & De-long diagram.[14][15]
Carbon & Nitrogen both are having significant role in controlling pure austenitic SS since it is strong austenite former. [Fig. 2] [Fig.3][20]

A study by R. H. Espy revealed that the effect of nitrogen on ferrite formation resulted in a decreased value of the nitrogen coefficient in the nickel equivalent.Espy suggested that the nitrogen coefficient be lowered from 30 to 20.[20]

It is also observed from the significance of each alloying elements graph That as Cr –equivalent Cr, Mo ,Si and Nb [fig.5][fig.10][fig.9][fig.8]

As a Ni –equivalent Ni, Mn, C, N and Cu are considered to be influential with delta ferrite. [fig.4][fig.2][fig.3][fig.6] in this connection, D; J. Kotecki and T. A.Siewert sought to include the effect of copper on the formation of ferrite in duplex stainless steels. While developing the WRC 1988 diagram, a copper coefficient was considered.[11]

The effect of Mn on ferrite content reducing content can also be observed with fig. (7). But according to E. R. Szurnachowski and D. J.Kotecki.[12]The effect of manganese on ferrite formation had been incorrectly established. An improved database revealed that the original 0.5 weighting factor should have been changed to unity (l), based upon work performed by them.

From the derived results, it can be concluded that the prediction of model is in tune with WRC-92 diagram's prediction. As can be observed in statistical summary the optimized model has correlation of 0.987168 as achieved between observed & predicted value.

This best trained Model not only exhibit the effect of individual alloying elements on Microstructure and Mechanical properties but also express the consequence, when act as an " individual" alloying element and in "combination". This study becomes very helpful in designing welding electrodes composition to achieve the desired resultant weld metal properties.

From the Fig. 2-10. It can be observed that Carbon Nitrogen & Manganese, copper & Nickel being a strong austenite former, have high influence on formation of ferrite content, whereas such influence can also be observed with Chromium, Molybdenum, Silicon & Niobium because of being strong Ferrite forming alloying elements.
Thus the prediction is in best tune with the different Cr- equivalent & Ni-equivalent mentioned in the different constitution diagrams as shown in table 7.

Table 7. Cr equivalents & Ni equivalents of respective constitution Diagrams.

Constitution Diagrams	Cr equivalent & Ni equivalent
Schaeffler Diagam (1949)	Cr eq = Cr + Mo + 1.5 Si +0.5 Nb Ni eq = Ni + 30C + 0.5 Mn
DeLong Diagram (1973)	Cr eq = Cr+Mo+1.5 Si + 0.5 Nb Ni eq = Ni + 30 C + 30 N + 0.5 Mn
WRC-92 Diagram (1992)	Cr eq = Cr + Mo + 0.7 Nb Ni eq = Ni + 35C + 20N + 0.25 Cu

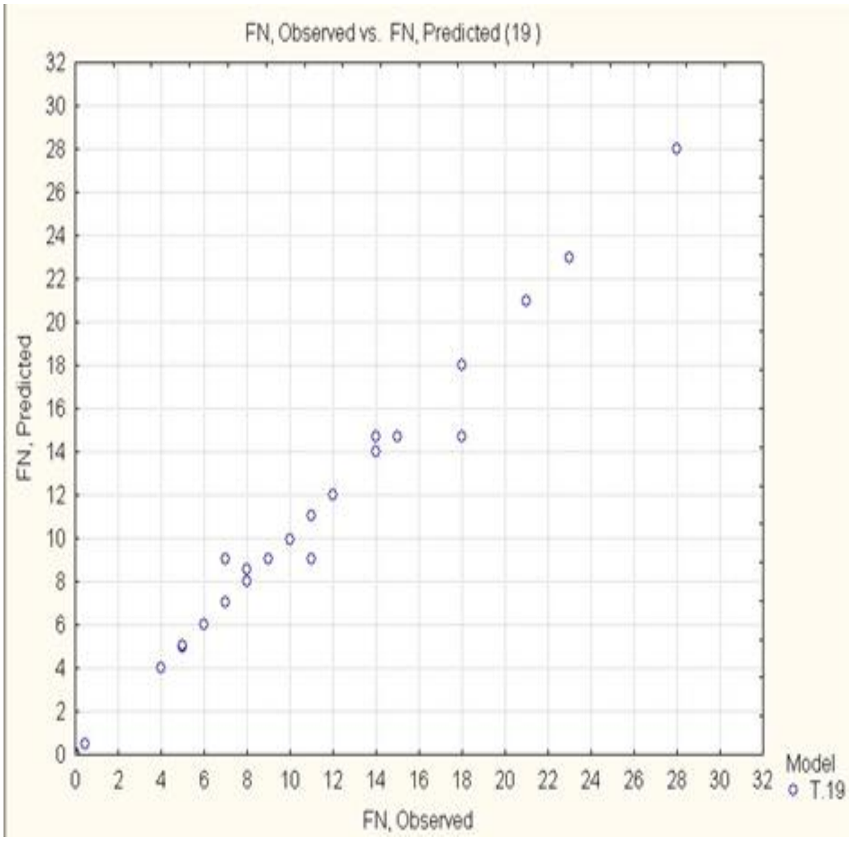

Fig. 1. Comparison between observed & predicted value of FN for an independent data set .Not used in the training. (16 dataset)

Table 8. The Summary of different three trained FN prediction models & their respective sum squared error for training data & Test data set.

FN PREDICTION METHODS	SUM SQUARED ERROR FOR COMPLETE TRAINING DATA SET	SUM SQUARED ERROR FOR INDEPENDENT (TEST) DATA SET
MLP 9:9-7-1:1	0.011343	0.032663
RBF 9:9-25-1:1	0.090368	0.0310
GRNN 9:9-116-2-1:1	0.018798	0.0041

A good conformity between the Observed & predicted values of Ferrite Number (FN) can be seen with the best optimized MLP 9:9-7-1:1 model, achieved with 0.987 index of correlation.

Table 9. Statistical analysis for observed & predicted values.

Data Mean	Data S.D.	Error Mean	Error S.D.	Abs E.Mean	S.D.Ratio	Correlation
6.675214	6.580961	0.050309	1.057986	0.414428	0.160765	0.987168

Conclusion

Having understood the potential effect of various alloying elements on the ferrite content in the weld metal, weld metal composition can be modified to control the desired level of ferrite content in the solidified weld deposits.

The model was trained on Austenitic stainless steel data which contained Ferrite number (FN) in range of 0 to 28. The prediction of FN for Duplex stainless steel data with higher value of FN between 40 to 50 was predicted with 0.98 correlations. This shows the excellent performance of NN modeling.

NN analysis can uncover the "trend" such as -when the X element in wt% added to steel the ferrite content can increase (OR decrease) but the underlying metallurgical fact can only be understood by physical experimentation and research.

In order to establish clear relations among various dependent and independent process parameters, a very accurate predictive tool calls for the more number of welding parameters.

Since neural networks take a considerable amount of time to train and physical validation is required to establish it more efficiently in real world applications.

Neural network is a powerful tool when complex relations between parameters cannot be modeled.

A neural network can predict trends and be in agreement with experimental data but
reliability of the predictions depends on the precision, size and preparation of the database.
Theory and mechanisms of the predicted parameters should be understood before analysis

Successfully trained NN model has been very useful tool for the cost reduction in the welding research field in the terms of material, money and time saving aspects in the sense that before doing physical experimentations by means of trialing and error methods, without involving in any cost, one can vary the input parameters and predict the output and go for designing various new weld alloys.

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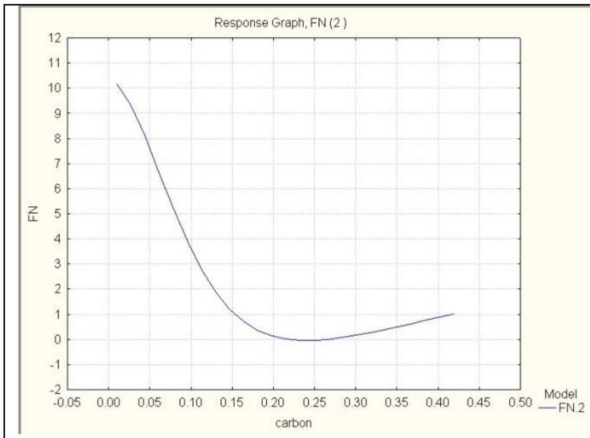

Figure 2 Effect of carbon on ferrite content

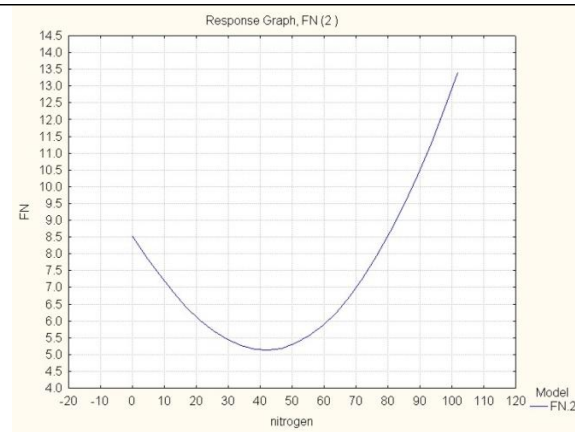

Figure 3 Effect of Nitrogen on ferrite content

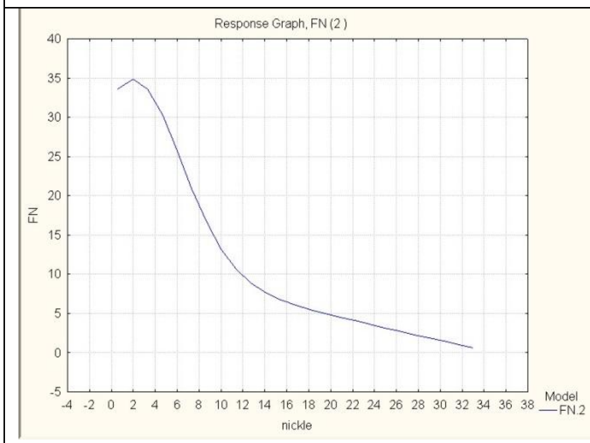

Figure 4 Effect of Nickel on ferrite content

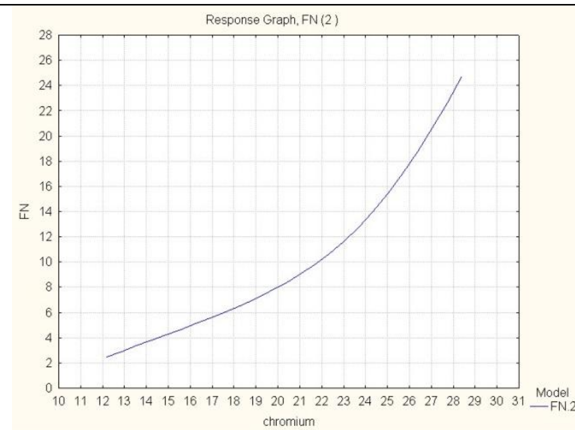

Figure 5 Effect of Chromium on ferrite content

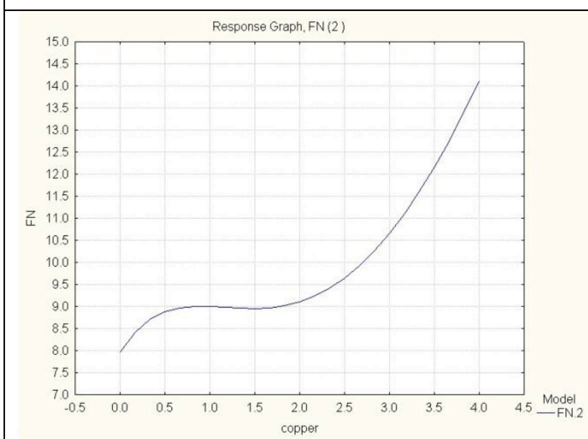

Figure 6 Effect of copper on ferrite content

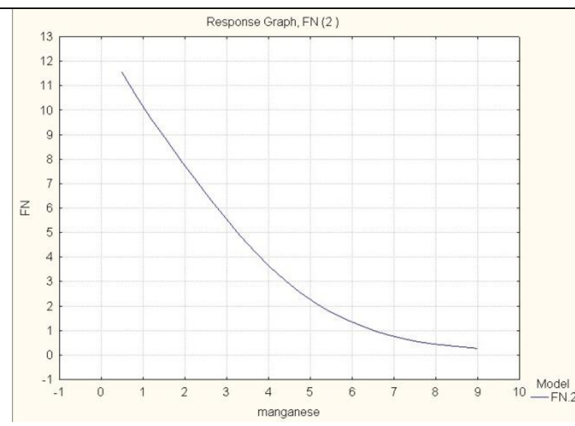

Figure 7 Effect of manganese on ferrite content

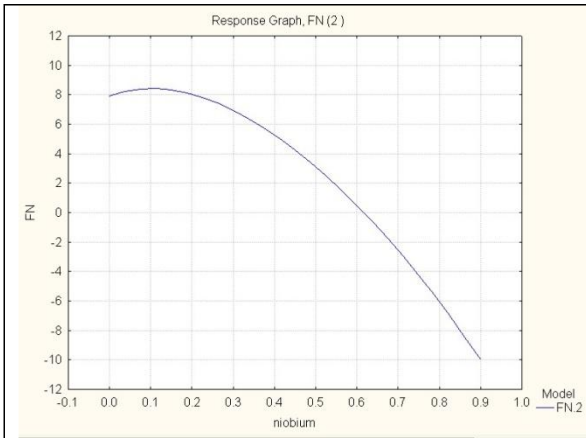

Figure 8 Effect of niobium of ferrite content

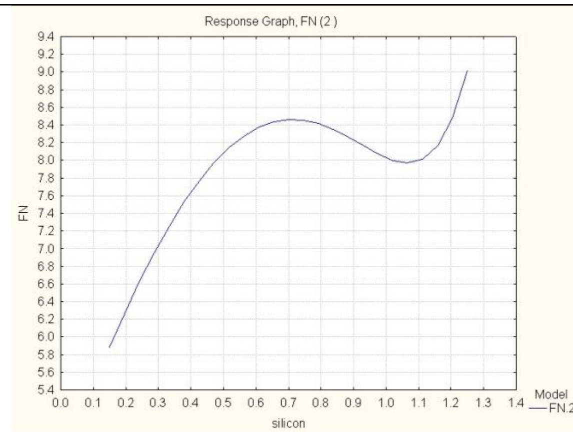

Figure 9 Effect of Silicon on ferrite content

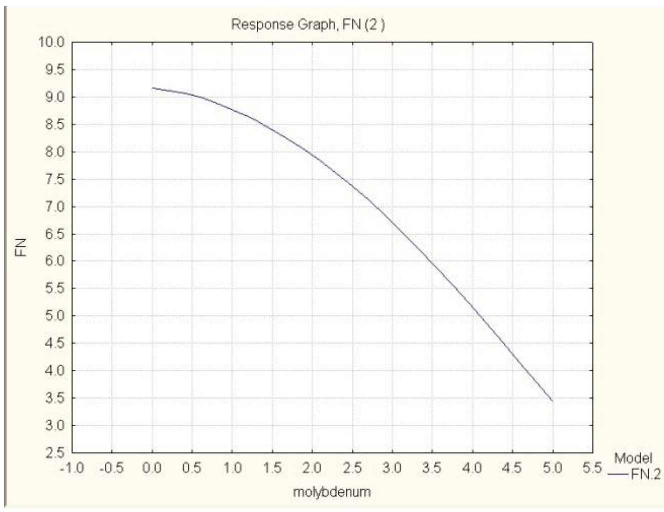

Figure 10 Effect of molybdenum on ferrite content

Fig. 2-10 Show the influence of individual alloying elements on ferrite content,
(Expressed in FN).

