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Contribution of Microalloying to the Strength of Hot-rolled Steels

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Abstract

Although the principles of microalloying are well-established, the complexity of thermomechanical processing is such that it is difficult to deconvolute the contribution to strength of the microalloying additions as a function of the many variables involved. We report in this paper the analysis of a large database on hot-rolled steels to create a neural network model which estimates the strength as a function of chemical composition and process variables. This model is then used to make comparisons against equivalent data in order to realise the role of minute additions of carbide formers in changing the properties of steels.

Keywords: microalloying, nonlinear analysis, strength, neural networks

1 Introduction

Microalloying has made a major contribution to the development of steels which help improve the quality of life through the better design of infrastructure. The principle is simple, that precipitates which are stable at high temperatures where steels are thermomechanically processed, serve to pin austenite grain boundaries [1]. This induces repeated recrystallisation of the austenite, and prevents its grain growth during hot-rolling, so that the fine austenite then transforms into correspondingly fine ferrite.

The strength of hot-rolled steels clearly must depend on thermomechanical processing and chemical composition, in particular the carbo-nitride forming elements niobium, vanadium and titanium, small concentrations (<0.10 wt%) of which both strengthen and toughen the standard carbon-manganese steels [1-4]. The purpose here was to interpret a large database in order to decipher the role of microalloying additions in modern steels with respect to strength. The problem is non-linear and best handled using a neural network. It is not the intention here to present the details of the technique itself, since this has been described elsewhere [5-9] and has been applied extensively in the context of steels [10-18].

2 Neural network

A hyperbolic tangent is a flexible, non-linear function, and combinations of different hyperbolic tangents allow mathematical functions which are able to capture empirical patterns in complex, multidimensional data. Such functions form the essence of neural networks. Their very flexibility, however, raises the possibility of overfitting data, a problem that can be avoided by using a randomly chosen sub-set (the training set) of the full set of available data. The part not used in creating the model, i.e., the test dataset, is then exploited in testing how the empirical fit generalises on unseen data. By ensuring that the model created represents both the training and test data equally well, it is possible to avoid overfitting.

There are two kinds of errors taken into account in the present work. The first is a noise, which represents the effect of missing variables, which is calculated as a constant value per model. The second is related to the fact that many empirical functions may adequately represent the same set of data, but which behave differently in extrapolation or interpolation. This modelling uncertainty is important in defining regions where the model is not firmly based on data. This is useful both in highlighting the danger of extrapolation and in defining regions of the input space where experiments are needed. Naturally, unlike the noise, the modelling uncertainty is a function of the position of input space where calculations are done.

2.1 Data

All of the data used have been provided by POSCO, based on experiments done on the tails of hot-rolled coils. Each experiment is associated with a value for the concentrations of carbon, manganese, silicon, phosphorus, sulphur, chromium, nickel, molybdenum, titanium, niobium, vanadium, aluminium, nitrogen, boron, copper, tin and calcium. In addition, the finish-rolling temperature (T_{FR}), coiling temperature (T_C), coil thickness (C_t), reheating time (t_R), reheating temperature (T_R) and total reduction ratio (reduction in thickness divided by the initial thickness ε_r) are specified. The statistical characteristics of the data are listed in Table 1.

2.2 Modelling

One hundred models were trained from which a committee of models which led to the smallest generalisation error was produced, and then retrained on the entire dataset without changing the complexity of any of the individual models. The details of these procedures have been described elsewhere [5,9] but the characteristics of the committee models for the ultimate tensile strength and yield strength are as follows:

Output	Noise σ_V	Number of models in committee
UTS σ_U	±0.014	3
Yield σ_Y	±0.040	4

The performance of the fully trained committee-models is illustrated in Fig. 1, and the ability of each input to explain variation in the output (*i.e.,* the significance) is shown in Fig. 2. As expected, C, Mn and Si correlate well with σ_U, as do the microalloying elements (Ti, Nb, V) even though they are added in small concentration. With the yield strength, the most significant variables are C, Mn, Si, Nb, C_t and ε_r. These outcomes will be discussed later in the text.

3 Analysis

In order to extract knowledge from the models, they were used to make predictions on the particular alloys listed in Table 2. Alloy A represents a mean set of parameters within the data used to create the models, whereas B, C and D correspond to reports in the literature, in order to test the role of microalloying additions [4,20,21]. When the full information was not reported with respect to the rolling schedule, it was assumed that the parameters corresponded to the mean values used here. When studying the effect of a particular variable, the remaining inputs were as listed in table 2. All the error bars represent the combined effect of the modelling uncertainty (±1σ) and noise of the committee model.

Nb, Ti and V carbonitrides prevent austenite grain coarsening during reheating and also help refine the austenite grain size during hot-rolling by pinning the grain boundaries and retarding recrystallisation [1,21]. By suppressing recrystallisation, they allow a higher fraction of the strain to be retained in the austenite. This increases the number density of ferrite nucleation sites, and finer ferrite grains are obtained after cooling. Nb is the most effective microalloying addition for suppressing the recrystallisation [3]. Many parts of this work are concentrated on the effect of Nb on the strengths.

Figure 3 shows the calculated effect of niobium on the strength of alloy B; experimental data due to [4] are also plotted for a niobium concentration of 0.023 wt%. It can be concluded that the 0.023 wt% addition has increased the yield strength by some 112 MPa but the ultimate tensile strength by only 46 MPa. The strength increment is of course useful but the difference between yield and ultimate strength has been dramatically reduced by the niobium addition which makes the steel less suitable for critical applications, such as earthquake-resistant steels, and where fatigue resistance is important [22]. Analysis of steel C, which is microalloyed with titanium, revealed a similar effect and the method accurately predicted the experimental data of [19] with calculated yield and UTS values being 450 and 542 MPa which compares with the measured values of 480 and 540 MPa respectively

(Fig. 4). This is in spite of the fact that steel C is not well-represented in the data used to train the model, resulting in large modelling uncertainties.

The greater sensitivity of the yield strength to microalloying is expected given that yield corresponds to the initial events leading to the propagation of slip across grain boundaries. On the other hand, the ultimate strength is associated with a large amount of plasticity and a work-hardened state, *i.e.,* when the microstructure has homogenised.

Figure 5 shows some interesting calculations designed to see the synergistic effects of microalloying with the combined additions of vanadium and niobium. They confirm that the yield strength is more sensitive to microalloying additions than the UTS. They further show that in steel A, an increase in the niobium concentration leads to strengthens the steel whereas the perceived effect of vanadium is small compared with the uncertainties to conclude that it is significant. In a series of studies, Medina and co-workers [23, 24] have shown that niobium is the most effective of microalloying elements in raising the static recrystallisation temperature of austenite, thus allowing more plastic strain to be retained before the austenite transforms into ferrite. The latter is therefore finer, thus adding to the strength of the steel. Similar results have been reported by Everett et al. [25]. Fig. 5 is consistent with these observations.

Fig. 6 shows a similar analysis with Ti and Nb as the microalloying additions. It is interesting that an increasing titanium concentration consistently leads to a reduction in the yield strength, and in general the UTS. Titanium is a stronger carbo-nitride former than niobium, and hence precipitates at a much higher temperature into relatively coarse particles, thus being less effective than niobium in raising the static recrystallisation temperature. Furthermore, its addition to a niobium-containing steel somewhat deprives the latter the opportunity to combine with interstitial elements and hence reduces the overall strength, making niobium less effective.

3.1 Heat Treatment and Rolling Temperatures

We have confirmed using the model that the strength of steel A hardly varies as a function of the reheating temperature over the range 1130-1250°C within the limits of uncertainty in the calculations. This is because the temperatures are all high enough to produce recrystallised austenite.

In the absence of microalloying, the yield strength decreases when rolling is finished at a high temperature (Fig. 7). This is not the case when a niobium addition is made because the T_{FR} is then below T_{nr}, which can be calculated using [26]:

$$T_{nr}\ /\ ^{\circ}\mathrm{C} = 887 + 464W_C + 890W_{Ti} + 363W_{Al} - 357W_{Si} + 6445W_{Nb}$$
$$-644\sqrt{W_{Nb}} + 732W_V - 230\sqrt{W_V}$$

where the concentrations of the elements (*W*) are in wt %. For steel A, T_{nr} is found to be 920°C meaning that pancaked austenite would be obtained for all T_{nr} below that temperature, consistent with Fig. 7 which shows that the strength of the Nb-containing alloy is insensitive to T_{FR}.

Fig. 8 shows that the properties of steel D are insensitive to the coiling temperature, and this is confirmed by the plotted experimental data from [27]. The insensitivity arises from the fact that the steels have a mixed microstructure of ferrite and pearlite, which completes transformation close to the eutectoid temperature (>700°C), so that the cooling subsequent to transformation does not influence the microstructure significantly. This would not be the case when lower temperature transformation products such as bainite are desired.

3.2 Model Validation

Data for further steels were collected from published results [4,19,28- 33]. Their chemical compositions are described in Table 3. These experimental results were used to demonstrate the predictive abilities of the models. The models are seen to work rather well (Fig. 9) on these data, for both microalloyed and steels which do not contain microalloying elements.

It is interesting that the model is able to generalise to data which evidently are out of the range used in the creation of the models. This statement is emphasised by the fact that the modelling uncertainties associated with the predictions in Fig. 9 are large (as would be the case for data out of the range of the training process), and yet the predictions are good. This indicates that the model has perceived physical relationships which are well-behaved on extrapolation.

4 Conclusions

It has been possible to create empirical models which are nonlinear and hence are able to capture the complex array of parameters which control the yield and ultimate tensile strengths of hot-rolled steels with a mixed microstructure of ferrite and pearlite. The method used is the neural network in a Bayesian framework. It is found without exception, that the model predictions are consistent with metallurgical observations and theories published in diverse sources.

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	Minimum	Maximum	Mean	St. Dev.
C / wt%	0.0012	0.8684	0.1009	0.0842
Mn / wt%	0.045	1.41	0.4763	0.2237
Si / wt%	0	1.954	0.0216	0.0594
P / wt%	0.003	0.11	0.0133	0.0055
S / wt%	0	0.017	0.0069	0.0025
Cr / wt%	0	0.46	0.0203	0.0266
Ni / wt%	0	0.44	0.0152	0.0239
Mo / wt%	0	0.2	0.0009	0.0044
Ti / wt%	0	0.058	0.0008	0.0035
Nb / wt%	0	0.041	0.0005	0.0026
V / wt%	0	0.041	0.0014	0.0018
Al / wt%	0	0.288	0.0319	0.0123
N / wt%	0	0.0087	0.0034	0.0014
B / wt%	0	0.0002	0.000026	0.000046
Cu / wt%	0	0.54	0.0098	0.0283
Sn / wt%	0	0.008	0.0019	0.0014
Ca / wt%	0	0.0032	0.0001	0.0004
T_{FR} / °C	700	930	867.3663	14.6396
T_C / °C	449	695	600.0074	26.9377
C_t / mm	1.4	12.7	4.76	2.56
t_R / min	116	903	205.7459	82.9132
T_R / C	1128	1247	1145.671	12.1482
Reduction	0.7214	0.9696	0.9039	0.0476
σ_U / MPa	292	1039	413.6963	71.9043
σ_Y / MPa	150	676	296.8	47.0699

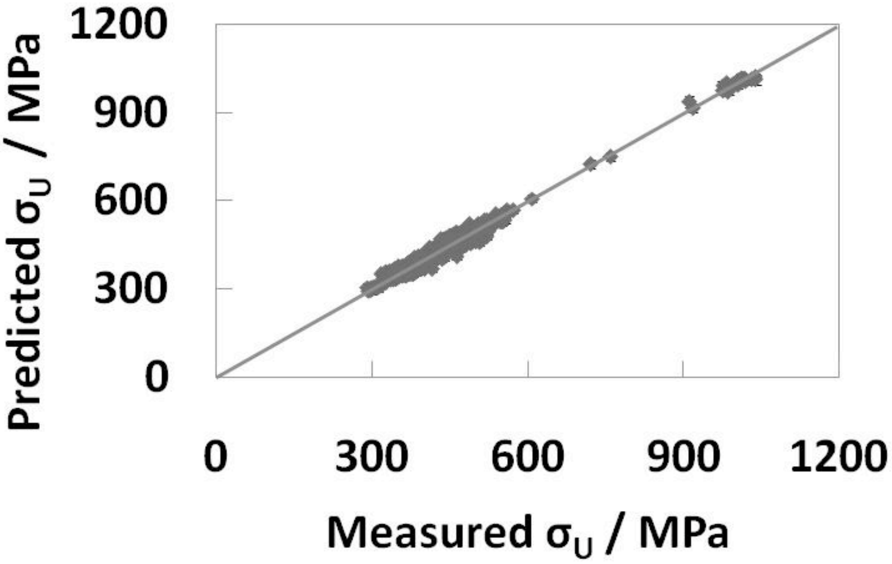
Table 1: Properties of data from 3385 experiments.

	A	B	C	D
C / wt %	0.1009	0.046	0.058	0.1
Mn / wt %	0.4763	1.19	0.52	0.91
Si / wt %	0.0216	0.03	0	0.01
P / wt %	0.0133	0.015	0	0.011
S / wt %	0.0069	0.002	0	0.008
Cr / wt %	0.0203	0	0	0
Ni / wt %	0.0152	0	0	0
Mo / wt %	0.0009	0	0	0
Ti / wt %	0	0	0.057	0.04
Nb / wt %	0.0005	0.023	0.054	0.03
V / wt %	0	0	0	0
Al / wt %	0.0319	0.038	0.052	0.04
N / wt %	0.0034	0.0067	0.0088	0.007
B / wt %	0.000026	0	0	0
Cu / wt %	0.0098	0	0	0.029
Sn / wt %	0	0	0	0
Ca / wt %	0	0	0	0
T_{FR} / °C	867	850	880	860
T_C / °C	600	450	600	520
C_t / mm	4.76	4.00	4.00	4.76
t_R / min	205	45	60	205
T_R / °C	1145	1100	1250	1150
ε_r	0.9039	0.88	0.87	0.9

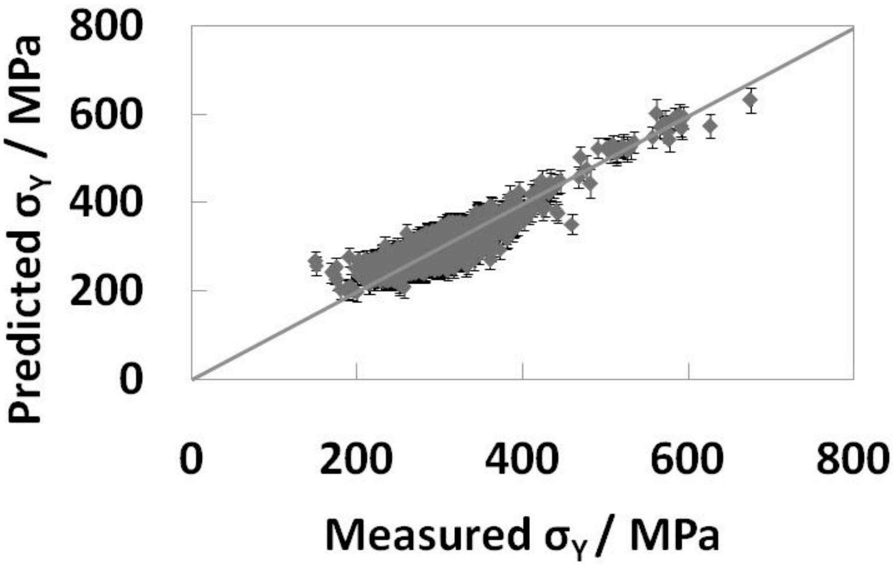
Table 2: Compositions of alloys used to study the effects of individual variables on the strengths

C	Mn	Si	P	S	Cr	Ni	Mo	Ti	Nb	V	Al	N	B	Cu	Sn	Ca
0.13	0.85	0.073	0.032	0.004	0	0	0	0	0	0	0.03	0.0038	0	0	0	0
0.12	1.34	0.044	0.021	0.001	0	0	0	0	0	0	0.033	0.003	0	0	0	0
0.1	1.2	0.79	0.013	0.001	0	0	0	0	0	0	0.043	0.003	0	0	0	0
0.312	1.51	0.27	0.021	0.008	0	0	0	0	0	0	0.029	0.0031	0	0	0	0
0.1	0.91	0.01	0.011	0.008	0	0	0	0.041	0.031	0.003	0.04	0.007	0	0.029	0	0
0.08	0.8	0.25	0.014	0.011	0	0	0	0	0	0	0.03	0	0	0	0	0
0.08	0.81	0.26	0.013	0.011	0	0	0	0	0.03	0	0.03	0	0	0	0	0
0.08	0.8	0.23	0.012	0.011	0	0	0.3	0	0.03	0	0.03	0	0	0	0	0
0.08	0.8	0.25	0.014	0.011	0	0	0.6	0	0.03	0	0.03	0	0	0	0	0
0.08	0.8	0.25	0.013	0.011	0	0	0.3	0	0	0	0.03	0	0	0	0	0
0.08	0.8	0.26	0.013	0.011	0	0	0.6	0	0	0	0.03	0	0	0	0	0
0.018	0.15	0.01	0.015	0.01	0	0	0	0	0	0	0.05	0.0035	0	0	0	0
0.0026	0.17	0	0.011	0.011	0	0	0	0.053	0	0	0.06	0.0013	0	0.008	0	0
0.0026	0.17	0	0.011	0.011	0	0	0	0.053	0	0	0.06	0.0013	0	0.008	0	0
0.025	1.56	0.24	0.002	0.0006	0	0	0.32	0	0.039	0.019	0	0.0062	0	0	0	0
0.049	1.45	0.51	0.014	0.002	0	0	0	0	0.025	0	0.047	0.0094	0	0	0	0
0.1	1.5	0.35	0	0.005	0	0	0	0	0	0.03	0.025	0.006	0	0	0	0
0.057	0.53	0	0	0	0	0	0	0	0	0	0.044	0.0046	0	0	0	0
0.052	0.52	0	0	0	0	0	0	0	0.019	0	0.035	0.0053	0	0	0	0
0.05	0.52	0	0	0	0	0	0	0	0.05	0	0.027	0.0053	0	0	0	0
0.055	0.52	0	0	0	0	0	0	0.019	0.052	0	0.046	0.0054	0	0	0	0
0.057	0.54	0	0	0	0	0	0	0.025	0.054	0	0.05	0.0062	0	0	0	0
0.058	0.52	0	0	0	0	0	0	0.057	0.054	0	0.052	0.0088	0	0	0	0
0.073	1.36	0	0	0.003	0	0	0	0	0.068	0	0.045	0.006	0	0	0	0
0.19	1.53	1.44	0	0	0	0	0	0	0	0	0	0	0	0.51	0	0
0.18	1.56	1.53	0	0	0.36	0	0	0	0	0	0	0	0	0.51	0	0
0.21	1.43	1.43	0	0	0	0.43	0	0	0	0	0	0	0	0.51	0	0
0.2	1.43	1.43	0	0	0.4	0.42	0	0	0	0	0	0	0	0.51	0	0

Table 3: Chemical compositions (wt %) to demonstrate the further ability of the models to generalise. The details of rolling schedule for the calculation are assumed to be the same as the mean values used here if they were missing in the literature.

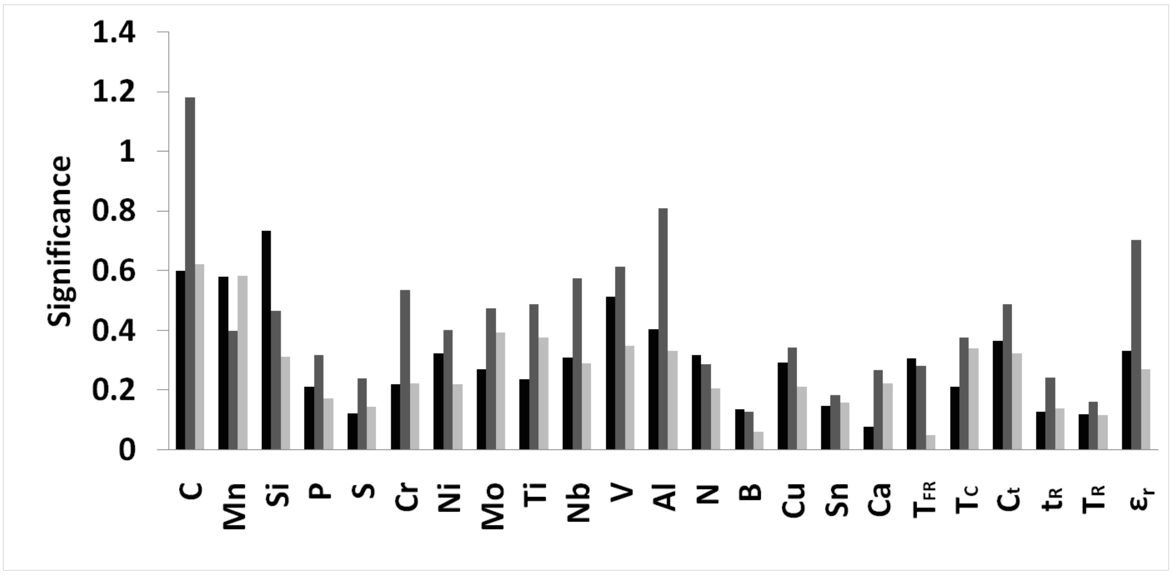


(a)

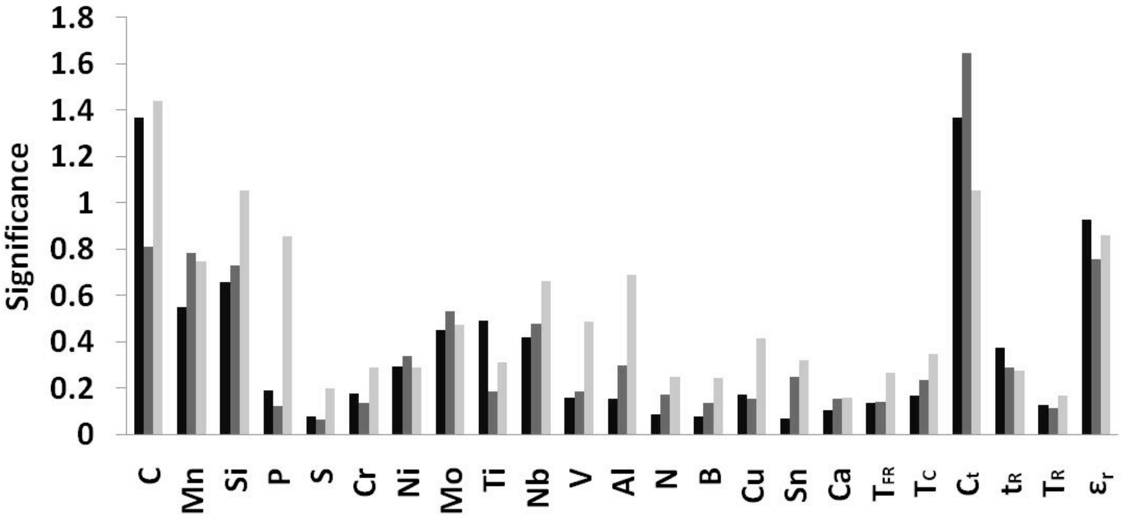


(b)

Figure 1: Comparison of measured and values calculated using the fully trained committee of models.



(a)



(b)

Figure 2: An illustration of the ability of each input to explain variation in the output (a) ultimate tensile strength (b) yield strength. Since committees of models are used, there are three values of significance illustrated for each variable corresponding to three members of each committee.

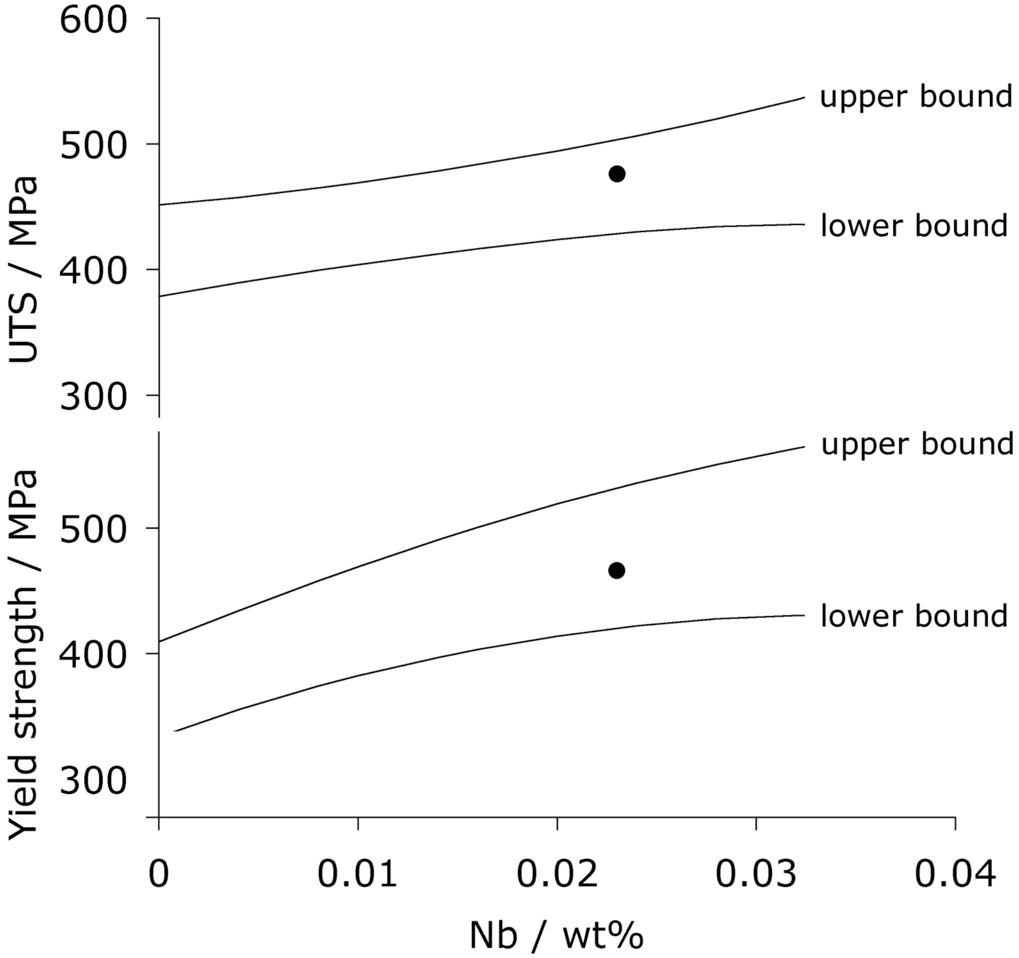


Fig. 3: Calculated curves showing the effect of niobium on strength of Alloy B. The points represent experimental measurements [4].

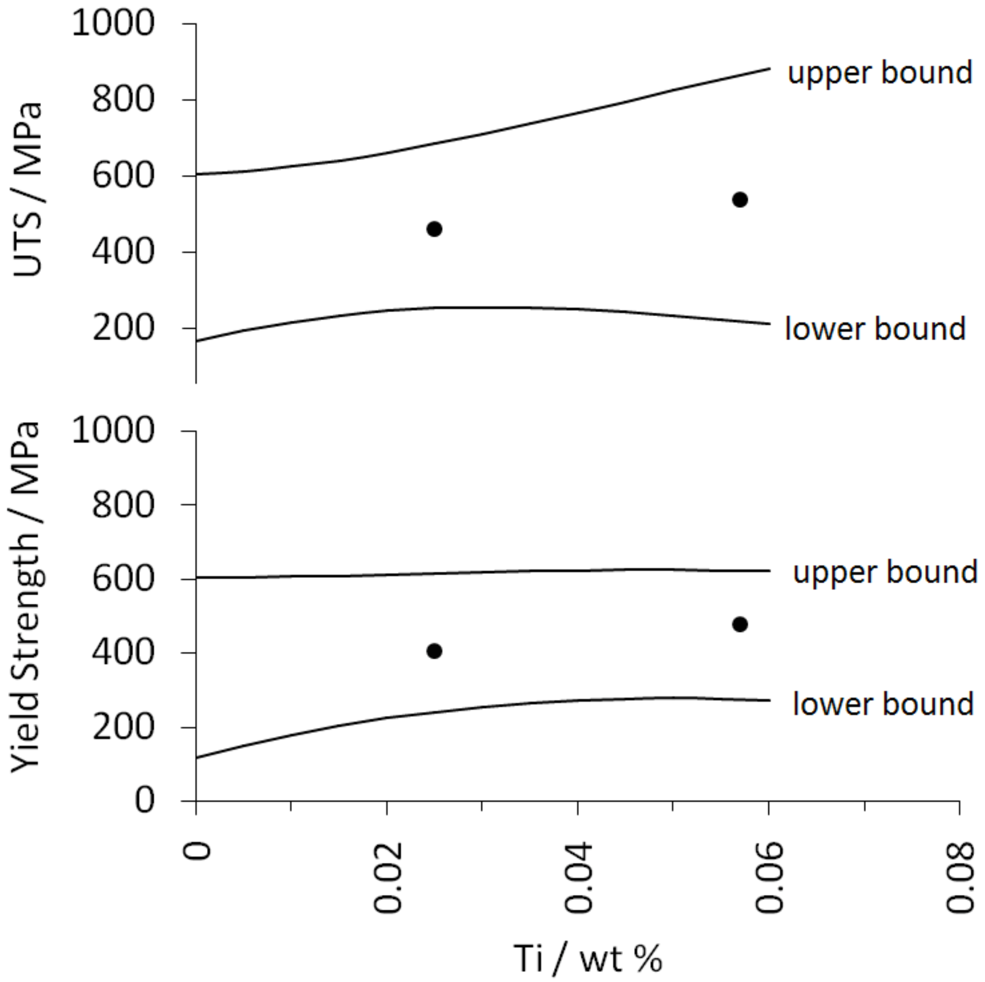


Fig. 4: Calculated curves showing the effect of titanium, on strength of Alloy C. The points represent experimental measurements [19].

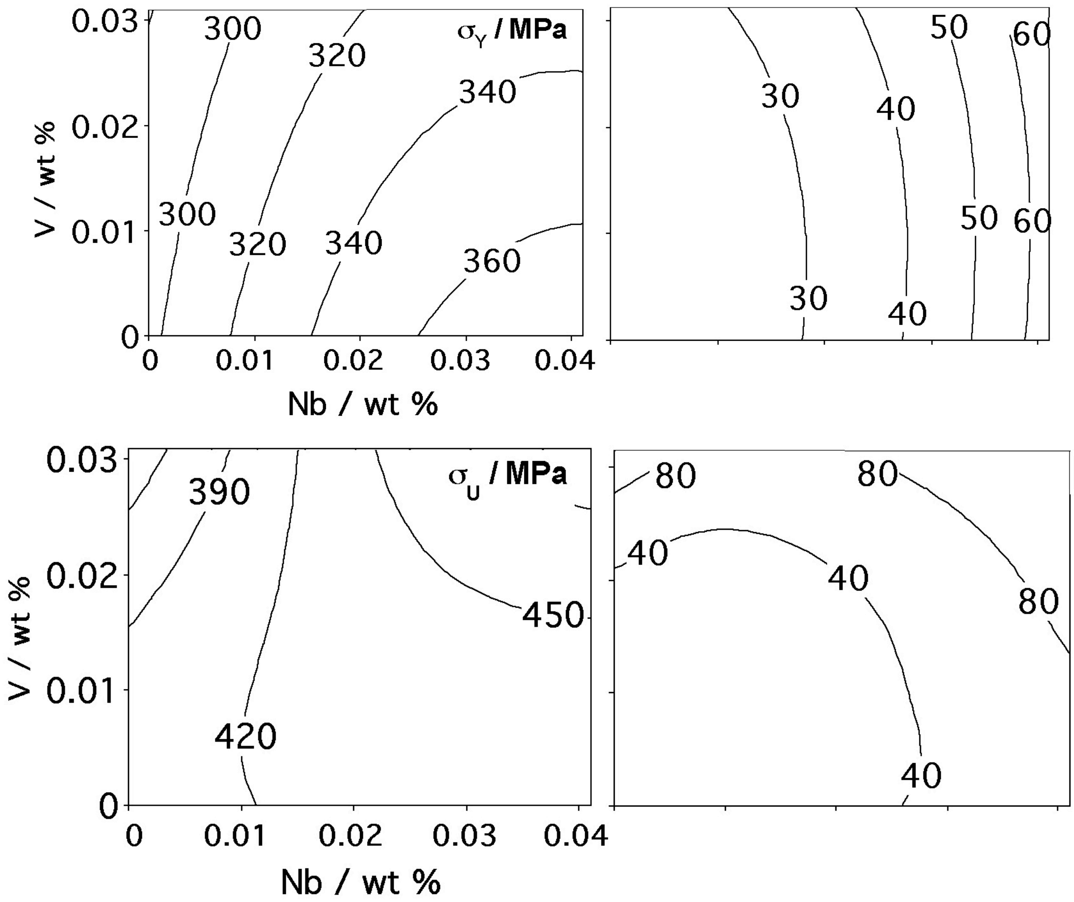


Fig. 5: Combined effect of vanadium and niobium on the properties of steel A. The plots on the right represent the uncertainties and are plotted to exactly the same scale as the plots on the left.

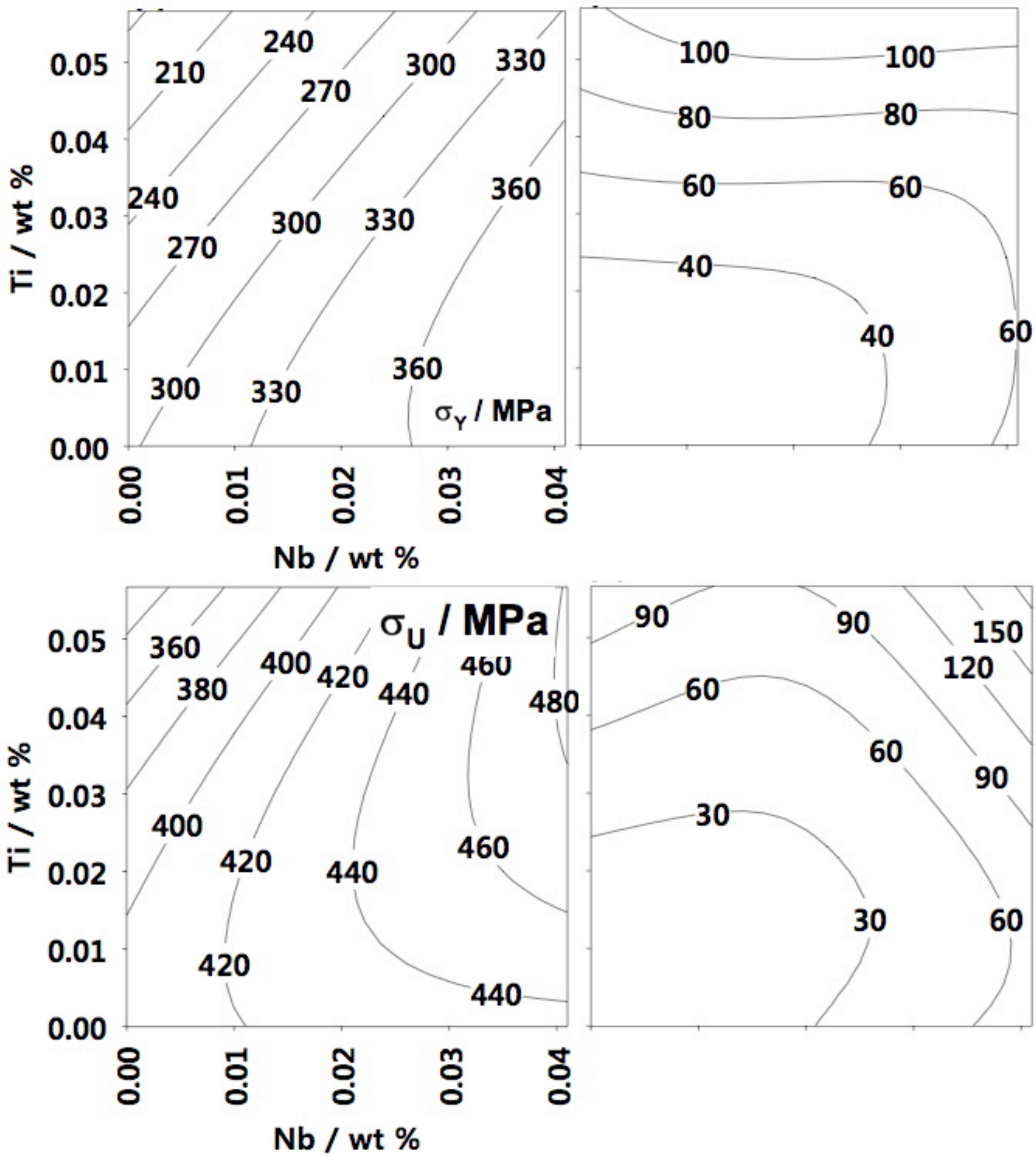


Fig. 6: Combined effect of titanium and niobium on the properties of steel A. The plots on the right represent the uncertainties and are plotted to exactly the same scale as the plots on the left.

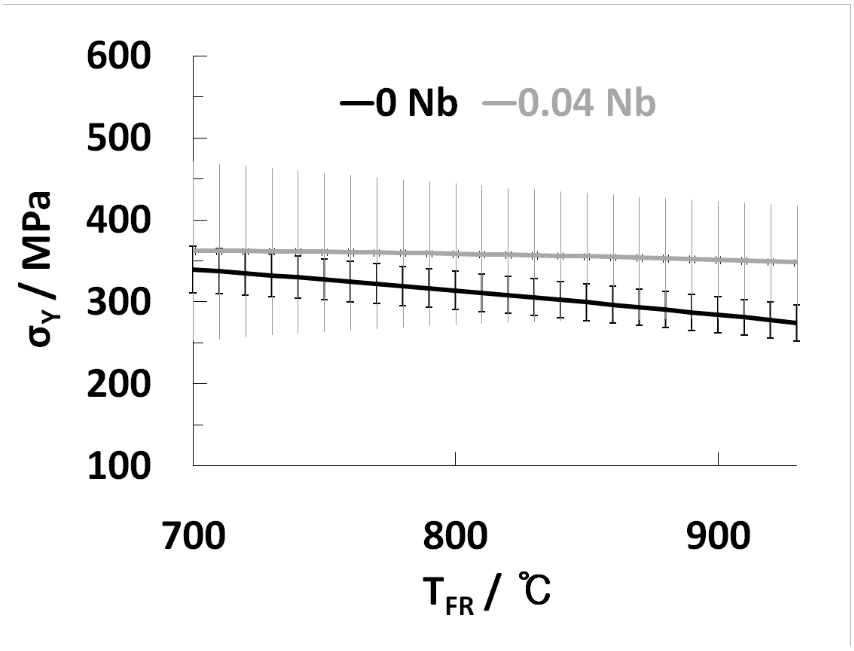


Fig. 7: Effect of finishing rolling temperature on the yield strength of alloy A.

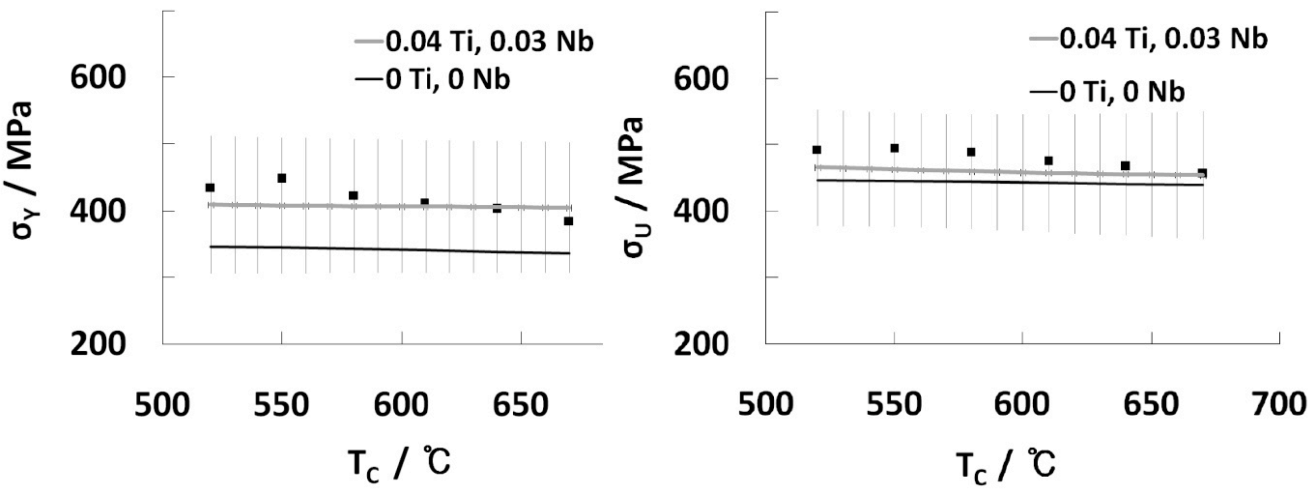


Fig. 8: Effect of coiling temperature on the strength of alloy D. The filled-square symbols represent experimental measurements [27].

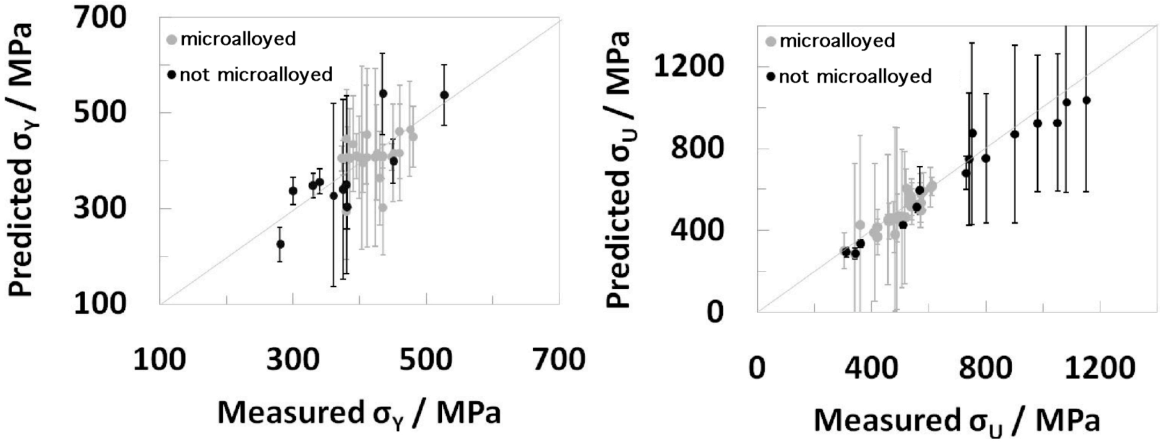


Fig. 9: Analysis of further data not included in the creation of the models.